Advanced Formulations and Applications of Finite Difference Time Domain Analysis

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Advanced Formulations and Applications of Finite Difference Time Domain Analysis

by

Ravi Chandra Bollimuntha

M.Tech., Banaras Hindu University, Varanasi, 2012

A thesis submitted to the

Faculty of the Graduate School of the

University of Colorado in partial fulfillment

of the requirements for the degree of

Doctor of Philosophy

Department of Electrical, Computer & Energy Engineering

2018
This thesis entitled:
Advanced Formulations and Applications of Finite Difference Time Domain Analysis
written by Ravi Chandra Bollimuntha
has been approved for the Department of Electrical, Computer & Energy Engineering

Prof. Melinda Piket-May

Prof. Mohammed Hadi

Date ____________________

The final copy of this thesis has been examined by the signatories, and we find that both the content and the form meet acceptable presentation standards of scholarly work in the above mentioned discipline.
This dissertation deals with advanced formulations and applications of finite difference time domain (FDTD) method. This is composed of four themes. The first deals with the development of a plane wave excitation formulation in FV24, a finite-volume based higher-order FDTD variant. With its excellent phase error performance even for coarse grid, FV24 can be applied to electrically large problems. The plane wave excitation method based on Total field/Scattered field formulation and Discrete planewave technique is demonstrated and validated for FV24. In the latter part of this work different near to farfield transformation approaches possible in FDTD are compared for accuracy.

The second part of the research deals with application of FDTD to glass weave-induced skew (GWS) problem. The GWS on a differential pair can cause increased bit error rates affecting the robustness of the digital system, and increased radiated emissions causing compliance failures. The frequency dependence of glass and resin materials properties are modeled using auxiliary differential equation formulation for FDTD, to estimate GWS on a differential pair. The skew numbers are benchmarked with the available commercial solvers. Also, the use of graphical processing units (GPUs) to accelerate the skew simulations is demonstrated.

The third part of the research deals with the derivation of numerical dispersion relation (NDR) for spherical FDTD, and the sensitivity study of the associated numerical wave number. Elementary functions native to spherical coordinates are used in the derivation of the numerical dispersion. Given the non-uniform nature of the spherical FDTD grid, the NDR and the corresponding numerical wave number are shown to be position dependent. The latter part of this research includes a study to derive the stability criterion for spherical FDTD and challenges involved therein.
The final part of the research studies the effectiveness of different absorbing boundary condition formulations for spherical FDTD in absorbing the waves. It is shown that the split-field formulation of perfectly matched layer (PML) is not as effective as stretched-coordinate formulation. This work includes derivation of continuous-space PML reflection coefficient, update equations for implementation of stretched-coordinate PML in spherical FDTD and analysis of reflection error for different PML parameters.
Dedication

In dedication to my mother Dhanalakshmi, my teachers and my wife Suganya Manoharan
Acknowledgements

Firstly, I would like to thank my advisers Prof. Melinda Piket-May and Prof. Mohammed Hadi and Prof. Atef Elsherbeni for their guidance and advice throughout my journey as doctoral student. Prof. Piket-May has been of constant support at every milestone from choosing the courses, preparing for the preliminary, comprehensive and final defense examinations. Many thanks to her patience and feedback while getting me ready for the conference presentations.

Special thanks to Prof. Mohammed Hadi for helping me shape the dissertation right from the beginning. This dissertation would not have been possible without his constant guidance, feedback, and availability for research reviews, and are greatly appreciated. His deep understanding of FDTD schemes, dedication to research, and attention to detail are motivational. Thanks to Prof. Atef Elsherbeni for his deep insights and feedback on the new formulations in the dissertation, and for his time for the research reviews despite his busy schedule. The FDTD codes from his text books have been tremendously helpful in quick implementation of the new formulations in this work.

I would like to thank Prof. Edward Kuester for being part of dissertation committee and for offering two wonderful courses: waveguides and transmission lines, and electromagnetic boundary problems. These courses helped me in not only understanding the theoretical basis, but are also instrumental in removing mathematical road blocks in my research - thanks to the rigorous and involved math in the courses. His clarifications on my research problems and feedback during the comprehensive exam are appreciated. His dedication to teaching is inspiring and commendable.

Thanks to Prof. Dejan Filipovic for guidance and support on securing teaching assistantship while he was the graduate director of the department. I am thankful for his kindness in lending
compute power and software licenses for my research. Thanks to Dr. Mohamed Elmansouri for agreeing to be on the committee in short notice. Working in the same lab, I observed him over four years, his dedication to research and guiding other students in the lab are inspiring.

Thanks to Dr. Eric Bogatin’s for the financial support and his high speed digital design course inspired me to think of application of FDTD method to practical problems such as glass weave induced skew dealt with in the thesis. His style of teaching, engineering and simulation philosophy influenced the way I approached my research. Thanks to Prof. Robert Marshall for interesting discussions on spherical perfectly matched layer and for sharing his equations and computer code on its implementation.

Thanks to Alpesh Bhobe, Soumya De, Mike Sapozhnikov and Amendra Koul from Cisco Systems Inc., and Kevin Zhu, David Fernandez at Ansys Inc. for discussions about my research during my internships. Thanks to research group members Alec Weiss, Ryan Smith, Sanjay Dmello, Vinit Vyas, Dharmateja Paladugu, Neeti Sonth, and fellow PhD students Tim Wang Lee and Fadi Deek for participating in numerous discussions about each other’s research and their feedback. Thanks to fellow graduate students Saurabh Sanghai, Prathap Valaleprasannakumar, Ehab Etellisi, Elie Tianang, Aman Samaiyar, Adbulaziz Haddab, and Prathamesh Pednekar for creating conducive atmosphere in the lab for research, their insight, advice and support.

I would like to thanks Adam Sadoff, Susan Callihan, Laramie Rose, Pamela Aguila, Kelly Payton, Christine Ralston in Dept. of ECEE for their administrative support and helping me navigate the graduate school, TA/RA appointment, and payroll paperwork.

Finally, I would like to thank my wife Suganya Manoharan for bearing with me patiently on numerous days while I conduct research and write thesis. Thanks to her helping hand in typesetting equations and being the first proofreader of the thesis draft. Her moral support and constant encouragement helped me in finishing my thesis on time.
Contents

Chapter

1 Introduction: Review of Finite Difference Time Domain Analysis  
1.1 Conventional FDTD  
1.2 Numerical Dispersion  
1.3 Field Sources in FDTD Grids  
1.4 Higher-Order FDTD: The FV24 Method  
1.5 Grid Truncation: Perfectly Matched Layer and Convolutional Perfectly Matched Layer  
1.6 Organization of Rest of the Chapters  

2 Planewave Injection in Higher-Order FDTD Grid  
2.1 Planewave Excitation in Standard FDTD  
2.1.1 Total Field/Scattered Field Formulation  
2.1.2 The Discrete Planewave Technique  
2.1.3 Auxiliary One-Dimensional Grid  
2.1.4 Properties of 1D Grid  
2.1.5 TF/SF Corrections  
2.2 Planewave Excitation in FV24 Grid  
2.2.1 FV24 Update Equations  
2.2.2 One-Dimensional Update Equations for FV24  
2.2.3 TF/SF Corrections for FV24
2.2.4 Waveform Excitation on 1D grid ........................................ 25
2.3 Validations of the Injection Technique ..................................... 29
2.4 Comparison of Near-to-Farfield Transformation Techniques for FDTD ......................................................... 30
  2.4.1 Arithmetic and Geometric Averaging .................................. 34
  2.4.2 The Separate and Mixed Surface Approach .......................... 35
2.5 Frequency Domain Near-to-Farfield Transformation in FDTD .......... 37
2.6 Error Comparison with a No Scatterer .................................... 38
  2.6.1 Resolution Sweep ...................................................... 39
  2.6.2 Incident Angle Sweep .................................................. 40
  2.6.3 Equivalent Surface Size Sweep ....................................... 41
  2.6.4 Bistatic RCS Comparison for a Dielectric Cube ..................... 42

3 Analysis of Glass Weave Induced Skew in Differential Pairs ............. 45
  3.1 Introduction: Glass Weave Skew in High Speed PCBs .................. 45
    3.1.1 FDTD Modeling of Glass-Resin Composites: Motivation .......... 49
    3.1.2 Implementation of Glass Weave Structure in FDTD Grid ........... 51
  3.2 Frequency Dependent Losses: Dispersive Medium ...................... 51
    3.2.1 Adapting Djordjevic-Sarkar Model to FDTD ........................ 53
    3.2.2 Implementation of Multi-Pole Debye Model in FDTD ............... 56
  3.3 Glass Weave Skew Analysis using FDTD .................................. 58
  3.4 Comparison with HFSS Simulations ..................................... 59
    3.4.1 Acceleration of FDTD in MATLAB ................................ 61

4 Spherical FDTD Dispersion Relation and Stability Analysis ............. 62
  4.1 Introduction to Spherical FDTD ........................................ 62
    4.1.1 Spherical FDTD Update Equations ................................. 63
  4.2 Numerical Dispersion Relation ......................................... 68
  4.3 Derivation of Spherical FDTD Numerical Dispersion Relation .......... 69
4.3.1 Position Dependence of Numerical Dispersion Relation ................................ 72
4.3.2 Convergence Analysis ....................................................................................... 72
4.4 Numerical Wave Number Sensitivity Analysis ....................................................... 73
4.4.1 Sensitivity to Mesh Resolution ........................................................................... 73
4.4.2 Sensitivity to Mode Numbers ............................................................................ 75
4.4.3 Sensitivity to Elevation Angle ........................................................................... 76
4.5 Stability Analysis .................................................................................................... 76
4.5.1 Existing Stability Analysis for Spherical FDTD .................................................. 78
4.5.2 Stability Criterion based on Position Dependent Numerical Dispersion Relation ................................................................. 79
4.5.3 Challenges in Validating Stability Criterion ....................................................... 82

5 Spherical FDTD PML Analysis ................................................................................. 83
5.1 Perfectly Matched Layer in Spherical FDTD ......................................................... 83
5.2 Split-Field PML Formulation ................................................................................ 84
5.3 Lossy Absorbing Shell as a Boundary Condition .................................................... 86
5.4 Stretched-Coordinate PML Formulation .............................................................. 88
5.4.1 Electric Field Stretched-Coordinate PML Equation ......................................... 88
5.4.2 Update Sequence .............................................................................................. 92
5.4.3 Magnetic Field Stretched-Coordinate PML Equation ...................................... 94
5.5 PML Reflection Analysis in Continuous Medium .................................................. 96
5.6 PML Performance Analysis ................................................................................... 98
5.6.1 Geometric Grading of PML Parameters ......................................................... 98
5.6.2 Simulation Space and Parameters ................................................................. 99
5.6.3 Performance Analysis and Comparison ............................................................ 101
5.7 Why Split-Field PML doesn’t work in Spherical FDTD? ........................................ 104
6 Conclusion

6.1 Original Contributions

Bibliography
## Tables

<table>
<thead>
<tr>
<th>Table</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Indexes for field location of S22 $E_x$ update equation</td>
<td>15</td>
</tr>
<tr>
<td>2.2</td>
<td>Indexes for field location of S22 $H_x$ update equation</td>
<td>16</td>
</tr>
<tr>
<td>2.3</td>
<td>Indexes for some field location of FV24 $E_x$ update equation</td>
<td>21</td>
</tr>
<tr>
<td>2.4</td>
<td>Indexes for some field location of FV24 $H_x$ update equation</td>
<td>22</td>
</tr>
<tr>
<td>3.1</td>
<td>Loss-less Material Properties</td>
<td>50</td>
</tr>
<tr>
<td>3.2</td>
<td>Material properties of glass and resin at 1 GHz</td>
<td>54</td>
</tr>
<tr>
<td>3.3</td>
<td>FDTD Simulation Parameters</td>
<td>58</td>
</tr>
<tr>
<td>4.1</td>
<td>Legendre Polynomials $P_n^m(\cos \theta)$ for some lower order $n$ and $m = 0$</td>
<td>75</td>
</tr>
<tr>
<td>5.1</td>
<td>Simulation parameters for PML/ABC implementations in spherical FDTD</td>
<td>100</td>
</tr>
<tr>
<td>5.2</td>
<td>Legendre Polynomials $P_n^m(\cos \theta)$ for some lower order $n$ and $m = 0$</td>
<td>104</td>
</tr>
</tbody>
</table>
Figures

Figure

1.1 Standard FDTD unit cell showing electric and magnetic field component locations

1.2 Computational voxel for FV24 algorithm vis-a-vis conventional FDTD unit cell

2.1 TF/SF formulation showing scatterer, total and scattered field regions, and interface surface between them

2.2 Auxiliary 1D grid, used in Discrete Planewave technique, in relation to the TF/SF formulation

2.3 The projections of E and H field locations are offset by $\Delta x/2$ on the 1D grid

2.4 A 2D view of the projections of E and H locations showing the uniformity of the 1D grid

2.5 Left: A set of $E_x$, $E_y$, and $E_z$ components having same projection on the 1D grid. Only a part of FDTD grid with $E$ component locations is shown. Right: A set of $H_x$, $H_y$, and $H_z$ components having same projection on the 1D grid. Only a part of FDTD grid with $H$ component locations is shown

2.6 Left: A 3D view showing projections of all $E$ and $H$ locations. Right: Another 3D view that shows several $E$ projections line up (similarly for $H$) forming a uniformly 1D grid

2.7 Computational voxel for FV24 algorithm vis-a-vis conventional FDTD unit cell
2.8 Left: Total Field $E_x$ (on Y planes) for which the whole H-plane (containing nine $H_z$ components) fall in scattered field region. Right: Total Field $E_x$ (that belong to X plane nodes or fall on Z planes of the TF/SF surface) for which only the three of the nine components on H-plane fall in scattered field region. Also included are the special cases at the corners. Respective incident $H$ fields need to be added to these H fields that fall in scattered field region. ........................................... 24

2.9 Left: 3D view of the Y planes, with blue and red being part of SF and TF respectively. Right: 2D view showing Scattered Field $E_x$ (on Y plane) for which the whole H-plane or part of it fall in total field region. Respective incident $H$ fields need to be subtracted from these H fields. .................................................. 25

2.10 Left: Scattered Field $E_x$ (on Z planes) for which part of the H-plane fall in total field region. Respective incident $H$ fields need to be subtracted from these $H$ fields. Right: Scattered Field $E_x$ (on X planes) for which part of the H-plane fall in total field region. Respective incident $H_z$ fields need to be subtracted from these $H$ fields. Also included are some special cases at the corners. ............................ 26

2.11 Scattered Field $E_x$ (diagonally outside the TF along the Y axis) for which part of the H-plane fall in total field region. Respective incident $H$ fields need to be subtracted from these $H$ fields. ................................. 26

2.12 Top: $E_x$ on 1D grid after 300 time-steps Bottom: $H_z$ on 1D grid after 300 time-steps 31

2.13 Top: Incident field $E_x$ in TF on a Z plane at the center of TF after 300 time-steps. Bottom: Incident field $H_z$ in TF on a Z plane at the center of TF after 300 time-steps. 32

2.14 Top: Leakage of $E_x$ into SF on a Z plane at the center of TF after 300 time-steps. Bottom: Leakage of $H_z$ into SF on a Z plane at the center of TF after 300 time-steps. 33

2.15 Schematic of the FDTD problem space, showing the dielectric scatterer, TF/SF regions and the Equivalent surface. .......................................................... 33

2.16 The tangential electric and magnetic fields on two separate surfaces, red and blue. 34
2.17 Left: Average of two Electric field components highlighted red. Right: Average of four Magnetic field components highlighted red. ................. 35

2.18 Left: Magnetic field-produced electric currents are placed on $S_e$. Right: Electric field-produced magnetic currents are placed on $S_h$ ................. 36

2.19 Maximum farfield error in dB for different grid resolutions. .......................... 39

2.20 Average farfield error in dB for different grid resolutions. .......................... 40

2.21 Maximum farfield error in dB for different plane wave incident angles. ............. 40

2.22 Average farfield error in dB for different plane wave incident angles. ............. 41

2.23 Maximum farfield error in dB for various equivalent surface sizes. ................. 41

2.24 Average farfield error in dB for various equivalent surface sizes. ................. 42

2.25 The $\theta$ component of bistatic RCS in different farfield planes. FDTD resolution is 40 cells/wavelength at 1 GHz. .......................... 44

3.1 Stack-up of a fourteen layer PCB [3], as an example. .......................... 46

3.2 Different glass weave styles and their style numbers. .......................... 46

3.3 A CAD model showing woven glass fiber and resin composite material. Also shown are glass-rich and resin-rich areas and a microstrip trace .......................... 47

3.4 A model showing two traces of a microstrip differential pair, one that falls entirely on glass fiber bundle and one that glass in between glass fiber bundles. ............. 48

3.5 Voltage waveforms show slight glass-weave induced timing skew on a differential a pair. .......................................................... 50

3.6 Glass fiber face modeled as an ellipse in $x - y$ plane as shown above and is swept along the $z$-axis modulating the $y$-coordinate of the center of the ellipse as shown below. .......................................................... 52

3.7 Various materials assigned to the cells in the FDTD grid modeling a PCB ............. 52

3.8 Multi-pole Debye model curve fitted to Djordjevic-Sarkar Modem for Glass and Resin materials. .......................................................... 55
3.9 Process flow showing sequence of steps involved in implementing dispersive FDTD.  

3.10 Pulse propagation on the differential pair obtained from FDTD simulation, and the timing skew between them.  

3.11 Top view of PCB Models for HFSS (left) and FDTD (right).  

3.12 Conversion of S-parameter data to time domain.  

3.13 Pulse propagation on the differential pair obtained from applying inverse Fourier transform to HFSS simulation results, and the timing skew between them.  

4.1 Spherical FDTD unit cell showing electric and magnetic field components’ locations.  

4.2 Spherical FDTD unit cell showing positional offsets of electric and magnetic field components.  

4.3 Edge lengths and face areas in spherical FDTD grid.  

4.4 A section of spherical FDTD grid showing discretization in r, θ, and φ directions.  

4.5 Special cells in spherical FDTD at poles and origin, also shown is a standard six-faced spherical FDTD unit cell.  

4.6 Numerical dispersion relation derivation process in general and steps involved in the derivation for Cartesian FDTD.  

4.7 Real and imaginary parts of wave number vs. normalized distance from origin at different resolutions (θ = Δθ, n = 3, and m = 0).  

4.8 Real and imaginary parts of wave number vs. normalized distance from origin for different mode numbers (θ = Δθ, R= 40, and m = 0).  

4.9 Real and imaginary parts of wave number vs. normalized distance from origin for different mode numbers m. Here θ = Δθ, R= 40, and n = 4.  

4.10 Real and imaginary parts of wave number vs. normalized distance from origin at different elevation angles (R = 40, n = 3, and m = 1).  

4.11 Problem space that excludes regions around origin to observe stability criterion practically for spherical FDTD.
4.12 Practically observed stability criterion for different PEC sphere radii and for different \( \Delta \theta \). .................................................. 81

4.13 Theoretical stability factor \( \tau \) at various PEC sphere radii for different modes \( n, m = 0 \). Also shown is the observed \( \tau \). .................................................. 81

5.1 PML boundary condition surrounding problem space in spherical FDTD. ............... 85

5.2 Spherical FDTD unit cell showing the field locations and their offsets. ................. 93

5.3 The position of PML region and PEC wall relative to origin. ............................... 97

5.4 Variation of conductivity \( \sigma_r \) in the PML region for different orders \( n_\sigma \) ........ 99

5.5 Problem Space for Spherical FDTD with PML ................................................... 100

5.6 Problem space for reference simulation in spherical FDTD ................................. 101

5.7 Comparison of Reflection Error for Split-Field PML and Absorbing Shell ABC for \( n_\sigma = 2 \) ................................................................. 102

5.8 Comparison of Reflection Error for stretched-coordinate PML for various PML poly-

5.9 Reflection Error for different mode numbers \( n \) and \( m = 0 \) in Continuous and FDTD

PML cases. ................................................................. 103
Chapter 1

Introduction: Review of Finite Difference Time Domain Analysis

This chapter introduces the finite difference time domain method and various tools associated with it that are used in later chapters. The finite difference time domain (FDTD) method introduced by Yee in [4] has been applied to a variety of electromagnetic wave (EM) problems. Numerous tools such as perfectly matched layer (PML) [5–8], auxiliary differential equation method [9, 10], plane wave excitation techniques [11–13], near to farfiled transformation [1, 14, 15], to name a few, have been developed to apply to various kinds of problems.

1.1 Conventional FDTD

The finite difference time domain method is an explicit formulation, i.e., there is no need for matrix inversions to solve a set of linear equations. In conventional FDTD, time domain Maxwell’s curl equations are discretized in both space and time using central difference scheme, producing second-order accurate update equations for electric and magnetic field components.

The FDTD unit cell in figure [1.1] [1] shows the positions of electric and magnetic field components. The update equations for $E_x$ and $H_x$ components are given in equations [1.1, 1.2] [1]. The update equations for $E_{y,z}$ are obtained from the update equation [1.1] for $E_x$ by replacing $x$ with $y$, $y$ with $z$, and $z$ with $x$.

The update equations for $H_{y,z}$ are obtained in a similar fashion from the update equation
1.2 Numerical Dispersion

Because of the discretization in space and time, the FDTD method doesn’t produce the same dispersion relation as that of free space, except for a special case in one dimension \[1\]. It implies that different frequencies will propagate with different velocities in the FDTD grid. The numerical dispersion relation for FDTD method is obtained by substituting plane wave solution in\[H_x\]. The complete FDTD update equation set can be found in \[1, 12\].

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

(1.1)

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

(1.2)
the update equations and reducing the resultant equations [1]. It is shown in equation (1.3)

\[ \mu \epsilon \left( \frac{\sin \omega \Delta t/2}{\Delta t/2} \right)^2 = \left( \frac{\sin \beta_x \Delta x/2}{\Delta x/2} \right)^2 + \left( \frac{\sin \beta_y \Delta y/2}{\Delta y/2} \right)^2 + \left( \frac{\sin \beta_z \Delta z/2}{\Delta z/2} \right)^2, \]  

where, \( \Delta x, \Delta y, \Delta z \) and \( \Delta t \) are spatial and temporal discretization steps, respectively. \( \omega \) is the angular frequency, and \( \beta \) is the numerical wave number. This relation also implies that the phase velocity of numerical waves in FDTD grid is direction-dependent (anisotropic) [12].

The numerical dispersion relation can be solved for numerical wave number \( \tilde{\beta} \). At low grid resolutions the numerical wave number in FDTD can be complex [12, 16] even for free space. The frequency spectrum of a wave being propagated in the FDTD grid can be wide containing low as well as high frequency components. For a given grid resolution, this might mean that the high frequency components are poorly resolved. This results in attenuation and faster-than-light (superluminal) propagation of these high frequency components [12].

Chapter 4 of this work deals with the derivation of numerical dispersion relation and analysis of numerical wave number for spherical FDTD (FDTD for spherical coordinates).

1.3 Field Sources in FDTD Grids

Sources are important in FDTD because they initiate the waves in the grid. Depending on the application, there are different kinds of sources we might want to implement in the FDTD grid, such as point-wise field sources, voltage and current sources, plane waves etc.

Pointwise field sources are the simplest to implement and are treated in [12, 17]. There are two flavors of field sources: a hard source and a soft source. The hard source is implemented by hard coding the field value at a point in the grid. For example, \( E_x^{n|_{(i,j,k)}} = f(n\Delta t) \) fixes the value of electric field component \( E_x \) to a particular value at every time step (at every instant \( n\Delta t \)) based on the choice of the source function \( f(t) \). As such, this component’s value at that location is not influenced by other field components surrounding it. As a consequence of this, hard source will reflect the wave coming towards it similar to a perfect electric conductor (PEC). On the other hand soft source doesn’t reflect and is transparent. It is implemented as
\( E_x^n(i,j,k) = \textbf{usual update equation} + f(n\Delta t) \), and the value of \( E_x^n(i,j,k) \) is influenced by other field components surrounding it because of the usual update equation involved. Comparing the soft source implementation to Maxwell’s curl equation with a current source, \( \nabla \times \mathbf{H} = \epsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{J} \), it is observed that the soft source is not actually a field source, but a current source.

The voltage and current sources can be implemented in the FDTD grid to excite a wave on a microstrip transmission line, for example. They can be lumped or distributed over a plane or a volume, and are dealt with in \([1, 18, 19]\). For voltage source implementation, the coefficients of the update equations are modified to include the internal resistance of the voltage source. And the voltage source term is added to the update equation as shown in equation 7b in \([18]\). Current sources are implemented in a similar fashion.

Plane wave sources, as the name implies, excite a plane wave in the FDTD grid and can be used to irradiate a scatterer to study its radar cross section, for example. Originally implemented by hard sourcing fields in the entire grid as an initial value problem by Yee \([4]\), this plane wave excitation has serious limitations \([12]\). Plane wave sourcing based on total field/scattered field formulation or pure scattered field formulation, which overcome these limitations, are discussed in \([1, 11–13, 20]\). Of these two, the total field/scattered field (TF/SF) formulation provides an excellent dynamic range for total fields as the scattered field formulation suffers form a phenomena called \textit{subtraction noise} \([12]\).

There are various techniques to calculate the incident fields required to implement TF/SF formulation. Incident field array (IFA) technique \([12]\) is based on auxiliary one dimensional grid and needs interpolation to calculate incident fields in the main grid. This increases field leakage into scattered field region and results in errors in scattering behavior \([12]\). One other technique to calculate incident fields is the auxiliary field propagator (AFP) technique \([20]\). While this method helps reduce spurious leakage into scattered field region, it needs expensive Fourier and inverse Fourier transforms to calculate incident fields at the TF/SF interface \([12]\). Moreover, it produces noncausal scattered field behaviour \([12]\). While this technique in its original form is not based on auxiliary 1D grid, its optimized version O-AFP \([21]\) is based on auxiliary 1D grid.
Discrete planewave (DPW) technique [22] based on 1D-MAP [13] methodology provides efficiency in calculation of incident fields and more than 300 dB of isolation between the total and scattered fields, thus drastically reducing the spurious leakage to machine precision levels.

Chapter 2 deals with implementation of the Discrete planewave technique for FV24, a finite-volumes based higher-order FDTD [23].

1.4 Higher-Order FDTD: The FV24 Method

Conventional or standard FDTD is second-order accurate method in both time and space. Many higher-order schemes are available in the literature for FDTD [24–27] either to control phase errors caused by numerical dispersion, or for better higher-order accuracy, or both [23]. Modified FDTD (2,4) or M24 [28] was introduced to model two-dimensional electrically large problems with high phase accuracy. Its three-dimensional counterpart is the finite-volumes based higher-order FDTD called FV24 [23]. They both are second order in time and fourth order in space algorithms.

The computational voxel or stencil for FV24 algorithm is shown in figure 1.2 [23]. While the stencil shown in the figure is for updating $E_x$, the other five stencils are similar. In addition to the four field components conventional FDTD considers, FV24 includes nine field components on each of the four parallel faces of a cube of size $3h \times 3h \times 3h$ as shown in figure 1.2. The cube is centered at the location of the field component that is being updated ($E_x$ in this case). The nine new field components are separated into three categorizes: $b$ for axial nodes, $c$ for surface axial nodes, and $d$ for surface diagonal nodes [23]. The contributions from these three categories are weighted differently in the update equations to account for their different radial distances. And these weights are optimized to minimize the phase errors [23].

Chapter 2 of this work deals with the plane wave excitation method for FV24.
1.5 Grid Truncation: Perfectly Matched Layer and Convolutional Perfectly Matched Layer

Effective truncation of FDTD grid without spurious reflections to simulate free space is of importance in open-region problems such as calculation of antenna radiation pattern or radar cross section (RCS) of a scatterer etc. In general, grid truncation can be classified into two classes: radiation boundary conditions (RBCs) and absorbing boundary conditions (ABCs). RBCs are based on analytical operators and many of them were introduced in the EM literature to emulate infinite free space. For a review of these methods, one can refer to [12]. They estimate the field value on the boundary using the known field values near the boundary based on differential operator (for example Sommerfeld radiation operator). While some advanced methods in this class can provide reflection errors down to -100 dB [12], they are suitable only to certain problems. The other methods in this class might not as effective in grid truncation as they suffer from spurious reflections.

The other class is the Absorbing boundary conditions (ABCs). An absorbing medium surrounds the main problem space in the directions where free space is required in a similar fashion to the absorbing material of an anechoic chamber, although physical taperings are often absent in numerical implementation. Early attempts as in [29] used a lossy, impedance-matched medium to
absorb waves and truncate the FDTD grid. However, it has limited application as the absorption is not effective for non-normal incident angle cases [12]. A more comprehensive ABC called the perfectly matched layer (PML), based on exploiting additional possibilities created by splitting the field components in Maxwell’s equation, was introduced by Berenger [5]. It is shown to be very effective in absorbing the waves in FDTD grid and other numerical techniques as well.

In continuous space, PML is reflection less, however the PML in FDTD is of finite thickness and is discretized, i.e., it is implemented as a multi-layered medium. This often results in spurious reflections. So, the PML parameters are geometrically graded to avoid reflections [12]. Later, PML has been re-interpreted as an uniaxial medium (UPML) by Gedney [6] and in stretched-coordinate form independently by Chew-Weedon [30] and Rappaport [31]. Complex frequency shifted PML (CFS-PML) [32, 33] was introduced to effectively absorb the evanescent modes that have long time interactions with PML. Its efficient implementation based on stretched-coordinate formulation called the convolutional PML (CPML) was introduced in [8]. Today, CPML stands as the effective way among ABCs to truncate FDTD.

Chapter 5 of this work deals with the implementation of PML for spherical coordinate FDTD.

1.6 Organization of Rest of the Chapters

This thesis is composed of four themes discussed in each of the next four chapters.

Chapter 2: The first theme deals with the development of a plane wave excitation formulation in FV24, a finite-volume based higher-order FDTD variant. With its excellent phase error performance even for coarse grid, FV24 can be applied to electrically large problems. The plane wave excitation method based on total field/scattered field formulation and Discrete Planewave technique is demonstrated and validated for FV24. In the latter part of this chapter different Near to Farfield transformation approaches possible in FDTD are compared for accuracy.

Chapter 3: The second part of the research deals with application of FDTD to an interesting problem encountered in printed circuit boards. The glass weave-induced skew in a differential
transmission line can cause a variety of problems as in increased bit error rates affecting the robustness of the digital system, and increased radiated emissions causing compliance failures etc. In this chapter, the auxiliary differential equation formulation for FDTD, that helps model frequency dependence of material properties of real materials, is used to estimate glass weave-induced skew in a differential pair. The skew numbers are benchmarked with the available commercial solvers. Also, the use of graphical processing units (GPUs) to accelerate the skew simulations is demonstrated.

Chapter 4: The third part of the research deals with the derivation of numerical dispersion relation for spherical FDTD, and the sensitivity study of the associated numerical wave number. Elementary functions native to spherical coordinates are used in the derivation of the numerical dispersion relation in contrast to plane waves used in the literature. Given the non-uniform nature of the spherical FDTD grid, the dispersion relation and the corresponding numerical wave number are expected and are shown in this work to be position dependent. The latter part of this chapter includes a study to derive the stability criterion for spherical FDTD and challenges involved therein.

Chapter 5: The final part of the research demonstrates the effectiveness of different absorbing boundary condition formulations for spherical FDTD in absorbing the waves without spurious reflections. It is shown that the split-field formulation of perfectly matched layer (PML) is not as effective in truncating the spherical FDTD grid as its stretched-coordinate formulation. This chapter includes derivation of continuous-space PML reflection coefficient, update equations for implementation of stretched-coordinate PML in spherical FDTD and analysis of reflection error for different PML parameters.
Chapter 2

Planewave Injection in Higher-Order FDTD Grid

Many electromagnetic wave (EM) applications involve a plane wave impinging on an object that can be either a receiving antenna or scatterers such as aircraft and ships in radar applications. Initiating a plane wave in a FDTD grid in order to simulate these real-life situations is of interest to the applied EM community, for example to estimate radar cross section (RCS) in radar applications or plot the radiation pattern of an antenna.

Different techniques exist for injecting this plane wave in a traditional FDTD grid, however the error-free and efficient technique has been the Discrete Planewave formulation [13,22].

In this chapter, we will show how this technique, which uses the total field-scattered field formulation to implement plane wave incidence, is implemented for a 3D finite volumes-based, extended-stencil FDTD (FV24) algorithm [23]. Its 2D version is M24 discussed in [28]. The FV24 method is based on the second-order in time and fourth-order in space finite-difference scheme whereas the conventional FDTD is obtained from second-order finite differences in both time and space. This method is designed to counter the effect of relatively large phase errors in propagated waves when a coarse grid is used [23] in modeling electrically large problems spanning hundreds of wavelengths. This work has also been published and available in [2].

Other tools available for FV24 are the convolutional perfectly matched layer (CPML) absorbing boundary conditions [34], conformal perfect electric conductor (PEC) modeling [35], and graphical processing units (GPU) code optimization [36].

Using the Discrete Planewave formulation, we can gain computational efficiency when the
three-dimensional FV24 grid is converted, exploiting the plane wave properties, into an auxiliary one-dimensional grid along the direction of plane wave propagation. The field leakage errors are eliminated through the dispersion-match between the one and three dimensional grids. As a consequence, the leakage errors into the scattered-field region are -300 dB below the incident field values and are observed to be independent of angle of incidence. This is a limitation set by the machine precision itself, not by the accuracy of the method.

Time-stepping along the aforementioned one-dimensional grid and the three-dimensional FV24 grid are run in parallel. The consistency corrections, needed for the update equations at the total field/scattered field boundary, are made using the field values from the one-dimensional grid. In contrast with the consistency corrections needed for plane wave incidence in traditional FDTD grid, more corrections are needed in FV24 grid due to its extended stencil. The complicated mapping between the corresponding field locations on the one-dimensional grid and the main three-dimensional grid will be demonstrated.

In the later part of the chapter, different interpolation schemes used in the process of transforming nearfields to farfields (near to farfield transformation) are compared.

2.1 Planewave Excitation in Standard FDTD

Planewave excitation technique in conventional FDTD based on an auxiliary one dimensional (1D) grid and total field/scattered field (TF/SF) formulation, as proposed by Tan and Potter \cite{13, 22} is reviewed first, and later will be extended to FV24 algorithm.

2.1.1 Total Field/Scattered Field Formulation

TF/SF formulation \cite{12} isolates the problem space into a total field and scattered field regions as shown in figure 2.1. The scattering object is placed inside the total field region and the virtual surface between the total field and scattered field regions is used to place fictitious electric and magnetic surface currents. These currents excite the required plane wave within the total field region, while allowing only scattered waves from the scatterer to pass through it. It is one of the
many flavors of the equivalence principle.

Figure 2.1: TF/SF formulation showing scatterer, total and scattered field regions, and interface surface between them [2].

2.1.2 The Discrete Planewave Technique

The Discrete Planewave method [13,22], which uses a 1D auxiliary grid that inherently propagates a plane wave with an identical numerical behavior as that of the main three dimensional grid, is the most effective TF/SF variant to date. The idea of auxiliary 1D in relation to TF/SF interface is shown in figure 2.2. The plane wave fields propagated on the 1D grid are mapped back to the main 3D grid and are used as fictitious surface currents on the TF/SF interface. This results in virtually no leakage of non-scattered fields outside the TF/SF interface -i.e., in scattered field region [2].

2.1.3 Auxiliary One-Dimensional Grid

The central theme behind implementing an error-free plane wave incidence using TF/SF formulation is the perfect numerical dispersion-matched 1D auxiliary propagator. In other words, the dispersion matching between the auxiliary 1D grid and the main FDTD grid makes it possible to reduce the spurious field leakage into the scattered field region to the order $10^{-15}$ or -300 dB below the field levels in total field region. The idea is to convert the same update equations as
that of the main 3D grid into 1D form for propagating the plane wave. This 1D implementation, as it becomes evident later in this section, is much more efficient than the 3D counterpart. For a 3D problem space, the FDTD update equations (consider equation 2.2 for example) operate on three dimensional E and H arrays. However, when we deal with a uniform plane wave, the same update equations can be modified so that they now involve operations on E and H that are just one dimensional arrays. This section will explain how this conversion (transformation or mapping) from 3D to 1D is done.

Every location, where either E or H field component is located in the main 3D FDTD grid, is projected onto an imaginary line in the direction of plane wave propagation. It is convenient to visualize this imaginary line as passing through the lower left corner of the TF region. The unit vector along this direction, in terms of the azimuth and elevation angles, is \( \mathbf{P} = \cos \phi \sin \theta \mathbf{a}_x + \sin \phi \sin \theta \mathbf{a}_y + \cos \theta \mathbf{a}_z \) or \( \mathbf{P} = p_x \mathbf{a}_x + p_y \mathbf{a}_y + p_z \mathbf{a}_z \).
As an example to demonstrate the projection mechanism, consider \( X = ((i+\frac{1}{2})\Delta x, j\Delta y, k\Delta z) \), the actual location of \( E_x \) associated with the node \((i\Delta x, j\Delta y, k\Delta z)\). The projection of this location along the imaginary line is \( P \cdot X = p_x\Delta x(i + \frac{1}{2}) + p_y\Delta yj + p_z\Delta zk \). If \( \frac{p_x\Delta x}{m_x} = \frac{p_y\Delta y}{m_y} = \frac{p_z\Delta z}{m_z} = \Delta r \) (the rational angle condition \([37]\)), for some odd integers \( m_x, m_y \) and \( m_z \), then \( P \cdot X = (m_xi + m_yj + m_zk + \frac{m_x}{2})\Delta r \). It means that this location’s projection is \( d = P \cdot X \) units from origin (the lower left corner of the TF region) along the imaginary line. Observe that the choice of \( m_x, m_y \) and \( m_z \) will decide the direction of plane wave propagation through the relations in equation 2.1 and theoretically infinite such directions are possible.

\[
\phi = \tan^{-1}\frac{m_y}{m_x}, \quad \theta = \cos^{-1}\frac{m_z}{\sqrt{m_x^2 + m_y^2 + m_z^2}} 
\] (2.1)

The collection of all the projections, of every \( E_{x,y,z} \) and \( H_{x,y,z} \) component location of the 3D main grid, forms the whole 1D grid. The projection’s distance from origin of 1D grid in terms of \( \Delta r \) is \((m_xi + m_yj + m_zk + \frac{m_x}{2})\), for example in the above case. This coefficient of \( \Delta r \) is generally a real number, however, it can be converted (as explained later) into an integer that can act as an index for the 1D electric and magnetic field arrays in computer memory.

Individual 1D grids can be formed by taking the projections of \( E_x \) locations alone (also applicable for \( E_{y,z} \) and \( H_{x,y,z} \)) as shown in 22. However, the term 1D grid refers to the whole 1D grid, formed from projections of all \( H_{x,y,z} \) and \( E_{x,y,z} \) locations on the 3D grid, in the rest of the paper unless pointed otherwise as individual. Although, we maintain six different 1D arrays for each of the six electric and magnetic field components that store the field values on respective individual 1D grids.

According to the property of the uniform plane wave that all the locations on a wave front have same phases and magnitudes, the projection of every point of the wave front onto the imaginary line is same (as the wave front is perpendicular to the direction of propagation). In other words, the \( E_x \) locations that have the same projection will have same field values at every instant. The same applies to \( E_{y,z} \) or \( H_{x,y,z} \). This property makes propagating a plane wave on 1D grid very attractive because of high memory and time efficiency 22 since we don’t need to store and perform
same update operations on exactly same field values (duplicates) repeatedly.

The conventional FDTD (standard second order in space and time or S22) update equation for $E_x$ in a loss-less homogeneous and isotropic medium, showing the exact field locations (half integer offsets), is given by equation 2.2. This equation operates on 3D arrays and can be converted into an update equation containing only 1D arrays (the 1D form) using the projections of the exact field locations in the 3D update equations.

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

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

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

(2.2)

However, as seen earlier, the projections are generally not integer multiples of $\Delta r$ making it difficult to use them directly as an index for 1D arrays in computer memory. If $m_x, m_y$ and $m_z$ are all odd integers, this problem can be rectified by simply adding $\frac{1}{2}$ to the non-integer coefficient of $\Delta r$ of the projection, i.e., the index on 1D grid of $E_x$ at location $((i + \frac{1}{2})\Delta x, j\Delta y, k\Delta z)$ on the 3D grid is $(m_xi + m_yj + m_zk + \frac{m_x}{2})$, for example.

However, care must be taken to avoid adding $\frac{1}{2}$ if a coefficient turns out to be integer by itself because of two fractions adding up. This happens for H components. For example, consider $H_z$ at $(i + \frac{1}{2}, j \pm \frac{1}{2}, k)$ or $H_y$ at $(i + \frac{1}{2}, j, k \pm \frac{1}{2})$ in equation 2.2 whose coefficients of projection distances are $\frac{d}{\Delta r} = I = (m_xi + m_yj + m_zk + \frac{m_x}{2} \pm \frac{m_y}{2})$ and $\frac{d}{\Delta r} = I = (m_xi + m_yj + m_zk + \frac{m_x}{2} \pm \frac{m_z}{2})$ respectively. These are already integers and can be used as index directly, i.e. there is no need to add corrective $\frac{1}{2}$ to coefficients of H component projections to extract a valid index $i$.

However, the above seemingly simple index extraction process for obtaining update equations in 1D form becomes complicated in practice, as it turns out that the only reference algorithm has, to choose right-hand-side $H_{y,z}$ components on the 1D grid, is the index of $E_x$, for example. So, we need to express the positions of $H_{y,z}$ components relative to this index (of $E_x$). For example, the projection of $H_z$ at $(i + \frac{1}{2}, j + \frac{1}{2}, k)$ is $(\frac{m_x}{2})\Delta r$ units away from the projection of $E_x$ on 1D grid. This relative distance, which is not an integer coefficient of $\Delta r$, is first converted into relative
index \( \frac{m_y+1}{2} \). Adding this to the corrected coefficient \( \frac{d}{Ar} = (m_x i + m_y j + m_z k + \frac{m_y+1}{2}) \) of \( E_x \) would have given the absolute index for \( H_z \). However, it doesn’t for the subtlety that we have over-estimated the index by correcting twice—the two halves add up and pick \( H \) at an unintended position. This can be rectified by adding \(-1\) to compensate, so the relative index for this \( H_z \) is

\[
i = (m_x i + m_y j + m_z k + \frac{m_y+1}{2} + \frac{m_y+1}{2} - 1) \quad \text{or} \quad i = (m_x i + m_y j + m_z k + \frac{m_y+1}{2} + \frac{m_y-1}{2}).
\]

Observe that we indeed would arrive at the same value directly from the projection of the location \( (i+\frac{1}{2}, j+\frac{1}{2}, k) \) of this \( H_z \), and can be used as consistency check (we would know this location beforehand by picturing the Yee grid in mind or by looking at the update equation, however, the algorithm can only deduce this by taking the location of \( E_x \) as reference and hence the rotund procedure). The projection of \( H_z \) at \( (i+\frac{1}{2}, j - \frac{1}{2}, k) \) is also \( (\frac{m_y}{2}) \Delta r \) away from the projection of \( H_x \) on 1D grid, however, on the opposite side on 1D grid. An integer index is obtained by subtracting \( \frac{m_y+1}{2} \) from the reference index of \( E_x \), i.e., \( I = ((m_x i + m_y j + m_z k + \frac{m_y+1}{2} - \frac{m_y+1}{2}) \). In this case as the two halves cancel rather than adding up, there is no need to compensate. Similar procedure can be followed to obtain \( H_y \) locations.

<table>
<thead>
<tr>
<th>Field Location</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E_x(i+\frac{1}{2},j,k) )</td>
<td>( m_x i + m_y j + \frac{1}{2} m_z k = K + \frac{m_y+1}{2} = ref )</td>
</tr>
<tr>
<td>( H_z(i+\frac{1}{2},j+\frac{1}{2},k) )</td>
<td>( K + \frac{m_z+1}{2} + \frac{m_y-1}{2} = ref + \frac{m_y-1}{2} )</td>
</tr>
<tr>
<td>( H_z(i+\frac{1}{2},j-\frac{1}{2},k) )</td>
<td>( K + \frac{m_z+1}{2} - \frac{m_y-1}{2} = ref - \frac{m_y-1}{2} )</td>
</tr>
<tr>
<td>( H_y(i+\frac{1}{2},j,k+\frac{1}{2}) )</td>
<td>( K + \frac{m_y+1}{2} + \frac{m_z-1}{2} = ref + \frac{m_z-1}{2} )</td>
</tr>
<tr>
<td>( H_y(i+\frac{1}{2},j,k-\frac{1}{2}) )</td>
<td>( K + \frac{m_y+1}{2} - \frac{m_z-1}{2} = ref - \frac{m_z+1}{2} )</td>
</tr>
</tbody>
</table>

The same approach is followed in order to convert the update equation 2.3 for \( H_x \), showing exact locations of the field components involved, into 1D from. The projection of \( H_x \) at \( (i, j + \frac{1}{2}, k + \frac{1}{2}) \) does not need any correction since \( \frac{d}{Ar} = (m_x i + m_y j + m_z k + \frac{m_y}{2} + \frac{m_z}{2}) \) is already an integer and used as index directly. Again, as the only reference that the algorithm has to choose \( E_{y,z} \) components on the 1D grid is the index of \( H_x \), we need to express the positions of \( E_{y,z} \) components relative to this index. For example, the projection of \( E_y \) at \( (i, j + \frac{1}{2}, k + 1) \) is \( (\frac{m_y}{2}) \Delta r \) away from
the projection of $H_x$ on 1D grid. This relative distance, which is not an integer coefficient of $\Delta r$, is converted into relative index $\frac{m_z+1}{2}$. Adding this to the coefficient $\frac{d}{\Delta r} = (m_x i + m_y j + m_z k + \frac{m_y}{2} + \frac{m_z}{2})$ of $H_x$’s projection, we get the index for this $E_y$ as $i = (m_x i + m_y j + m_z k + \frac{m_y}{2} + \frac{m_z}{2} + \frac{m_z+1}{2})$. The projection of $E_y$ at $(i, j + \frac{1}{2}, k)$ is also $(\frac{m_z}{2})\Delta r$ away from the projection of $H_x$ on 1D grid, however, on the opposite side on 1D grid. Subtracting $\frac{m_z+1}{2}$ from the index of $H_x$ would result in a integer $(m_x i + m_y j + m_z k + \frac{m_y}{2} + \frac{m_z}{2} - \frac{m_z+1}{2})$. However, it would become evident after consistency check that we under-estimated the index and so a compensatory 1 is added. Finally, the correct integer index for this $E_y$, i.e. $I = (m_x i + m_y j + m_z k + \frac{m_y}{2} + \frac{m_z}{2} - \frac{m_z-1}{2})$. The summary of indexes for all field components in S22 update equations for $E_x$ and $H_x$ are listed in tables 2.1 and 2.2, respectively.

\begin{align*}
H_x^{n+\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) &= H_x^{n-\frac{1}{2}}(i, j + \frac{1}{2}, k + \frac{1}{2}) \\
&+ \frac{\Delta t}{\mu \Delta y} \left[ E_y^n(i, j + \frac{1}{2}, k + 1) - E_y^n(i, j + \frac{1}{2}, k) \right] \\
&- \frac{\Delta t}{\mu \Delta z} \left[ E_z^n(i, j + 1, k + \frac{1}{2}) - E_z^n(i, j, k + \frac{1}{2}) \right] \quad (2.3)
\end{align*}

Table 2.2: Indexes for field location of S22 $H_x$ update equation

<table>
<thead>
<tr>
<th>Field Location</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_x(i, j + \frac{1}{2}, k + \frac{1}{2})$</td>
<td>$m_x i + m_y j + m_z k + \frac{m_y}{2} + \frac{m_z}{2} = K + \frac{m_y}{2} + \frac{m_z}{2} = ref$</td>
</tr>
<tr>
<td>$E_y(i, j + \frac{1}{2}, k + 1)$</td>
<td>$K + \frac{m_x}{2} + \frac{m_y}{2} + \frac{m_z+1}{2} = ref + \frac{m_z+1}{2}$</td>
</tr>
<tr>
<td>$E_y(i, j + \frac{1}{2}, k)$</td>
<td>$K + \frac{m_x}{2} + \frac{m_y}{2} - \frac{m_z-1}{2} = ref - \frac{m_z-1}{2}$</td>
</tr>
<tr>
<td>$E_z(i, j + 1, k + \frac{1}{2})$</td>
<td>$K + \frac{m_x}{2} + \frac{m_y}{2} + \frac{m_z+1}{2} = ref + \frac{m_z+1}{2}$</td>
</tr>
<tr>
<td>$E_z(i, j, k + \frac{1}{2})$</td>
<td>$K + \frac{m_x}{2} + \frac{m_y}{2} - \frac{m_z-1}{2} = ref - \frac{m_z-1}{2}$</td>
</tr>
</tbody>
</table>

2.1.4 Properties of 1D Grid

If all the space is meshed (i.e. not confining ourselves to the truncated region of interest) and projections of all possible 3D locations of $E$ and $H$ components are taken on the imaginary line along the direction of plane wave propagation, and are sorted (in ascending order) after eliminating the duplicates, we will have a uniformly spaced discrete set of points, the so called 1D grid, along the
imaginary line. Because of the inherent spatial offset (staggered in space) of $E$ and $H$ components in the FDTD grid (it is assumed that the $E$ components are edge centered while $H$ components are face centered), the projections of $E$ components are $d = (m_xi + myj + m_zk)\Delta r + \frac{m_{x,y,z}\Delta r}{2}$ (non-integer multiple of $\Delta r$) and of $H$ components will be either $d = (m_xi + myj + m_zk)\Delta r + \frac{(m_x+m_z)\Delta r}{2}$, or $d = (m_xi + myj + m_zk)\Delta r + \frac{(m_x+m_y)\Delta r}{2}$ or $d = (m_xi + myj + m_zk)\Delta r + \frac{(m_x+m_y)\Delta r}{2}$ (integer multiple of $\Delta r$).

Let the projection of $H$ component associated with some node $(i_1,j_1,k_1)$ be $d = n\Delta r$ for some integer $n$, and for a given combination of $(m_x,m_y,m_z)$. It is interesting to observe that there is another node $(i_2,j_2,k_2)$ whose associated $E$ component’s projection is $d = n\Delta r + \frac{\Delta r}{2}$. The consequence of the observation is that the 1D grid is uniform and has a spacing of $\frac{\Delta r}{2}$ with alternate $E$ and $H$ component projections. This property of the 1D grid is shown in figure 2.3.

Figure 2.4 offers a 2D view of projections of $E$ and $H$ locations and shows the uniformity of the 1D grid.

Also, the electric field components $E_x$, $E_y$, or $E_z$ can have same projection. For example, consider $m_x = 5$, $m_y = 3$ and $m_z = 1$. This combination makes the the projections of $(i+\frac{1}{2},j,k+2)$, $(i,j+\frac{3}{2},k)$, and $(i,j+1,k+\frac{3}{2})$, the 3D locations of $E_x$, $E_y$ and $E_z$ components respectively, co-located on the 1D grid as shown in figure 2.3. Similar observation can be made for $H$ components as well. Figure 2.6 offers a 3D view of projections of $E$ and $H$ locations. It also shows a 3D view that displays how several $E$ projections, displayed by solid lines, line up and fall at a set of locations on the imaginary line. Similarly, several $H$ projections, displayed by dotted lines, line up and fall
at another set of location on the imaginary line. These sets of projections form the 1D grid and the $E$ and $H$ projections on it alternate.

Figure 2.5: Left: A set of $E_x$, $E_y$ and $E_z$ components having same projection on the 1D grid. Only a part of FDTD grid with $E$ component locations is shown. Right: A set of $H_x$, $H_y$ and $H_z$ components having same projection on the 1D grid. Only a part of FDTD grid with $H$ component locations is shown.

### 2.1.5 TF/SF Corrections

In FDTD grid, the surface currents are introduced at the TF/SF interface by means of consistency corrections to the field update equations [12], and are detailed in section 2.2.3.
Figure 2.6: Left: A 3D view showing projections of all $E$ and $H$ locations. Right: Another 3D view that shows several $E$ projections line up (similarly for $H$) forming a uniformly 1D grid.

2.2 Planewave Excitation in FV24 Grid

In this section, we will demonstrate the plane wave excitation method discussed above for FV24 algorithm.

2.2.1 FV24 Update Equations

The computational voxel (stencil) for FV24 algorithm is shown in figure 2.7. While the stencil shown in figure 2.7 is for updating $E_x$, the other five stencils are similar. In addition to the four field components conventional FDTD considers, FV24 includes nine field components on each of the four parallel faces of cube of size $3h \times 3h \times 3h$ centered at the location of the field component that is being updated ($E_x$ in this case.)

The FV24 update equation for $E_x$ is as follows:

\[
E_x^{n+1}(i + \frac{1}{2}, j, k) = E_x^n(i + \frac{1}{2}, j, k) \\
+ cb1x \left[ H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{1}{2}, k) - H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j - \frac{1}{2}, k) \right] \\
+ cb2x \left[ H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{3}{2}, k) - H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j - \frac{3}{2}, k) \right] \\
+ cb3x \left[ H_z^{n+\frac{1}{2}}(i + \frac{3}{2}, j + \frac{3}{2}, k) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j + \frac{3}{2}, k) \right]
\]
\[
+ H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{3}{2}, k + 1) + H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j + \frac{3}{2}, k - 1)
\]
\[
- cb3x \left[ H_z^{n+\frac{1}{2}}(i + \frac{3}{2}, j - \frac{3}{2}, k) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j - \frac{3}{2}, k) \right]
\]
\[
+ H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j - \frac{3}{2}, k - 1) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j - \frac{3}{2}, k - 1) \]
\[
+ cb4x \left[ H_z^{n+\frac{1}{2}}(i + \frac{3}{2}, j + \frac{3}{2}, k + 1) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j + \frac{3}{2}, k + 1) \right]
\]
\[
+ H_z^{n+\frac{1}{2}}(i + \frac{3}{2}, j + \frac{3}{2}, k - 1) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j + \frac{3}{2}, k - 1) \]
\[
- cb4x \left[ H_z^{n+\frac{1}{2}}(i + \frac{3}{2}, j - \frac{3}{2}, k + 1) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j - \frac{3}{2}, k + 1) \right]
\]
\[
+ H_z^{n+\frac{1}{2}}(i + \frac{3}{2}, j - \frac{3}{2}, k - 1) + H_z^{n+\frac{1}{2}}(i - \frac{1}{2}, j - \frac{3}{2}, k - 1) \]
\[
- cb1x \left[ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j + \frac{1}{2}, k - \frac{1}{2}) - H_z^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{1}{2}) \right]
\]
\[
- cb2x \left[ H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k + \frac{3}{2}) - H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j, k - \frac{3}{2}) \right]
\]
\[
- cb3x \left[ H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j + 1, k + \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j - 1, k + \frac{3}{2}) \right]
\]
\[
+ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j, k + \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i - \frac{1}{2}, j, k + \frac{3}{2}) \]
\[
+ cb3x \left[ H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j + 1, k - \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i + \frac{1}{2}, j - 1, k - \frac{3}{2}) \right]
\]

b – axial H nodes

c – surface axial H nodes
d – surface diagonal H nodes

Figure 2.7: Computational voxel for FV24 algorithm vis-a-vis conventional FDTD unit cell.
$+ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j, k - \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i - \frac{1}{2}, j, k - \frac{3}{2})]$

$- cb4x \left[ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j + 1, k + \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i - \frac{1}{2}, j + 1, k + \frac{3}{2}) \right]$

$+ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j - 1, k + \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i - \frac{1}{2}, j - 1, k + \frac{3}{2}) \right]$

$+ cb4x \left[ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j + 1, k - \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i - \frac{1}{2}, j + 1, k - \frac{3}{2}) \right]$

$+ H_y^{n+\frac{1}{2}}(i + \frac{3}{2}, j - 1, k - \frac{3}{2}) + H_y^{n+\frac{1}{2}}(i - \frac{1}{2}, j - 1, k - \frac{3}{2}) \right]. \quad (2.4)$

2.2.2 One-Dimensional Update Equations for FV24

Similar to the conventional FDTD, integral based FV24 FDTD update equation can be reduced to 1D form. Consider the FV24 update equation (2.4) for $E_x$, for which the indexes of some field locations are listed in Table 2.3. The indexes for rest of the field locations can be constructed based on those listed in the table. Similarly, for the FV24 update equation of $H_x$, the indexes of some field locations are listed in Table 2.4.

Table 2.3: Indexes for some field location of FV24 $E_x$ update equation

<table>
<thead>
<tr>
<th>Field Location</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_x(i + \frac{1}{2}, j, k)$</td>
<td>$m_xi + m_yj + m_yk + \frac{m_y+1}{2} = K + \frac{m_y+1}{2} = ref$</td>
</tr>
<tr>
<td>$H_z(i + \frac{1}{2}, j + \frac{3}{2}, k)$</td>
<td>$K + \frac{m_y+1}{2} + \frac{3m_y-1}{2} = ref + \frac{3m_y-1}{2}$</td>
</tr>
<tr>
<td>$H_z(i + \frac{1}{2}, j - \frac{3}{2}, k)$</td>
<td>$K + \frac{m_y+1}{2} - \frac{3m_y+1}{2} = ref - \frac{3m_y+1}{2}$</td>
</tr>
<tr>
<td>$H_z(i + \frac{3}{2}, j + \frac{3}{2}, k + 1)$</td>
<td>$K + \frac{m_y+1}{2} + m_x + \frac{3m_y-1}{2} + m_z = ref + m_x + \frac{3m_y-1}{2} + m_z$</td>
</tr>
<tr>
<td>$H_z(i + \frac{1}{2}, j - \frac{3}{2}, k - 1)$</td>
<td>$K + \frac{m_y+1}{2} - m_x - \frac{3m_y+1}{2} - m_z = ref - m_x - \frac{3m_y+1}{2} - m_z$</td>
</tr>
</tbody>
</table>

2.2.3 TF/SF Corrections for FV24

The six E and H update equations converted to 1D form (that manifest the 1D propagator) are run along with the time stepping of the main FV24 grid. That is, at each time step, we update E and H at every location on the 1D grid first and then on the main grid later. The TF/SF corrections are required for the consistency of main grid’s update equations at the Huygens surface which acts
Table 2.4: Indexes for some field location of FV24 $H$ update equation

<table>
<thead>
<tr>
<th>Field Location</th>
<th>Index</th>
</tr>
</thead>
<tbody>
<tr>
<td>$H_x(i, j + \frac{1}{2}, k + \frac{1}{2})$</td>
<td>$m_xi + m_yj + m_yk + \frac{m_x}{2} + \frac{m_y}{2} = K + \frac{m_x}{2} + \frac{m_y}{2} = ref$</td>
</tr>
<tr>
<td>$E_y(i, j + \frac{3}{2}, k + 2)$</td>
<td>$K + \frac{m_y}{2} + \frac{m_z}{2} + m_y + \frac{3m_z+1}{2} = ref + m_y + \frac{3m_z+1}{2}$</td>
</tr>
<tr>
<td>$E_y(i, j - \frac{1}{2}, k - 1)$</td>
<td>$K + \frac{m_y}{2} + \frac{m_z}{2} - m_y - \frac{3m_z-1}{2} = ref - m_y - \frac{3m_z-1}{2}$</td>
</tr>
<tr>
<td>$E_y(i + 1, j + \frac{3}{2}, k + 2)$</td>
<td>$K + \frac{m_y}{2} + \frac{m_z}{2} + m_x + m_y + \frac{3m_z+1}{2} = ref + m_x + m_y + \frac{3m_z+1}{2}$</td>
</tr>
<tr>
<td>$E_y(i - 1, j - \frac{1}{2}, k - 2)$</td>
<td>$K + \frac{m_y}{2} + \frac{m_z}{2} - m_x - m_y - \frac{3m_z-1}{2} = ref - m_x - m_y - \frac{3m_z-1}{2}$</td>
</tr>
</tbody>
</table>

as a boundary between the total field and the scattered field regions (the Huygens surface itself is assumed to be part of total field region and contains some E and H field locations as was done in [12]).

Consider the main grid’s update equation for an $E_x$ falling on the boundary (the Huygens surface that belongs to total field). This will have some of the right-hand side $H_y$ and $H_z$ falling in total-field region and some in scattered field region making the update equation for this $E_x$ inconsistent. The $H$ fields falling in the scattered field region need consistency corrections, i.e., we need to convert them to total fields by adding the incident $H$ fields at those respective locations as shown in equation 2.5. The incident $H$ fields are present on the 1D grid, more specifically, in the three 1D arrays for $H_x$, $H_y$ and $H_z$ which have been computed already. Based on the location of the main grid’s $H$ field that needs correction, we construct the index by calculating its projection on the 1D grid, then pick the $H$ field value on the 1D grid at that index and add it to correct the main grid’s $H$ field.

$$E_x^{n+1}|_{tot} = E_x^n|_{tot} \pm \{H_z^{n+\frac{1}{2}}|_{tot} \pm \{H_z^{n+\frac{1}{2}}|_{scat} + H_z^{n+\frac{1}{2}}|_{inc} \pm \{H_y^{n+\frac{1}{2}}|_{scat} + H_y^{n+\frac{1}{2}}|_{inc} \} \} \quad (2.5)$$

In contrast with the consistency corrections needed for plane wave incidence in S22 grid, we need far more corrections here in FV24 grid. Consistency corrections are needed even for some $E_x$ fields falling in the scattered field region (the case not present for S22). For these locations, we will have some of the right-hand side $H_y$ and $H_z$ falling in total-field region and some in scattered field region. This will make the update equation for $E_x$ inconsistent. The total $H$ fields are to be converted to scattered fields by subtracting the incident $H$ fields in order to make the update...
The equation consistent as shown in equation 2.6

\[
E_{x}^{n+1}|_{\text{scat}} = E_{x}^{n}|_{\text{scat}} \pm \{H_{z,y}^{n+\frac{1}{2}}|_{\text{tot}} - H_{z,y}^{n+\frac{1}{2}}|_{\text{inc}}\} \pm \{H_{y}^{n+\frac{1}{2}}|_{\text{tot}} - H_{y}^{n+\frac{1}{2}}|_{\text{inc}}\}
\]  

(2.6)

In the rest of the section we highlight the corrections to be made to the \(H_{z}\) fields of the \(E_{x}\) update equation at locations where it becomes inconsistent. Similar correction methodology can be applied for \(H_{y}\) components of \(E_{x}\) update equation and further to rest of the five update equations.

The six faces of TF/SF (Huygens) surface are \(i = i_{0}, i = i_{1}, j = j_{0}, j = j_{1}, k = k_{0}\) and \(k = k_{1}\) and they correspond to the terminating YZ, XZ and XY planes (or simply X, Y and Z planes) respectively.

First, consider the corrections to the \(E_{x}\) that fall on/inside the total field (TF) region. The \(E_{x}\) locations that are on the two Y planes, i.e. \(j = j_{0}\) and \(j = j_{1}\), need similar corrections. This is because, for each one of these \(E_{x}\) locations, one of the two H-planes that contains the nine \(H_{z}\) components falls completely in the scattered field (SF) region. To be more precise, for each of the \(E_{x}\) on \(j = j_{0}\), the H-plane that is at \(j = j_{0} - \frac{3}{2}\) is completely in SF as shown in figure 2.8: left, where as for the \(E_{x}\) on \(j = j_{1}\), the H-plane that is at \(j = j_{1} + \frac{3}{2}\) is completely in SF. So, the respective incident \(H_{z}\) fields, picked from the 1D grid’s \(H_{z}\) (1D array) after forming the index for each of the nine main grid’s \(H_{z}\) locations, are added to the right hand side of the \(E_{x}\) update equation.

Also, for the \(E_{x}\) that fall inside the TF on \(j = j_{0} + 1\) and \(j = j_{1} - 1\), one of the H-planes falls completely in SF region, also shown in figure 2.8: left, and similar corrections as the above case are needed.

The \(E_{x}\) locations that are on the Z planes \(k = k_{0}, k_{1}\) and that belong to the nodes on X planes \(i = i_{0}, i = i_{1}\) of the TF/SF cubic-boundary, there are \(H_{z}\) fields falling in both TF and SF as shown in figure 2.8: right. Again, those falling in SF need consistency corrections, i.e. the incident \(H_{z}\) fields at these locations available on the 1D grid need to be added the RHS of the main grid’s \(E_{x}\) update equation.

Second, consider the corrections to the \(E_{x}\) that fall outside the total field (TF) region. For the \(E_{x}\) locations that are part of the Y plane \(j = j_{0} - 1\)(which is in SF) shown in figure 2.9: Left,
some or all of the \( H_z \) fall in the total field (TF) region and are highlighted in figure 2.9 Right. So, the \( E_x \) update equation at each of these SF locations are inconsistent and the incident \( H_z \) fields on the 1D grid at the indexes corresponding to these highlighted main grid’s locations need to be subtracted from the RHS of the main grid’s \( E_x \) update equation. similar corrections are needed for the \( E_x \) falling on Y plane \( j = j_1 + 1 \).

The corrections needed for the update equation at \( E_x \) locations that either fall on Z planes \( k = k_0 - 1, k = k_1 + 1 \) or that belong to the nodes on X planes \( i = i_0 - 1, i = i_1 + 1 \) are shown in figure 2.10 Almost all the locations on the above Z planes (or all \( E - x \) locations that belong to the above X planes) have similar corrections with exceptions only at corners.

Lastly, the \( E_x \) that are located diagonally outside the TF and along the Y-axis, i.e. those falling on the lines formed by the intersection of plane-pairs \( k = k_0 - 1 \& i = i_0 - 1, k = k_0 - 1 \& i = i_1, k = k_1 + 1 \& i = i_0 - 1 \) and \( k = k_1 + 1 \& i = i_1 \) as shown in figure 2.11 may have a lone
Figure 2.9: Left: 3D view of the Y planes, with blue and red being part of SF and TF respectively. Right: 2D view showing Scattered Field $E_x$ (on Y plane) for which the whole H-plane or part of it fall in total field region. Respective incident $H$ fields need to be subtracted from these H fields.

$H_z$ falling inside TF. This inconsistent update equation can be made consistent by subtracting the incident $H_z$ field picked from the 1D grid.

### 2.2.4 Waveform Excitation on 1D grid

In order to initiate a waveform on the 1D grid, the first few nodes of it are hard wired at every time step using either analytical expressions for E and H (analytic source method), or Optimized AFP (O-AFP) \[21\]. For both the methods, the dispersion relation given by equation 2.7 is solved using a root-finding technique to find the numerical wavenumber $\tilde{k}$. The procedure to populate fields at initial nodes on the 1D grid is similar in both the methods. Given a time series $f(n)$ at a reference point on 1D grid, use the numerical wavenumber $\tilde{k}$ to delay $f(n)$ appropriately and find the incident field time series $f_{E,H}(n)$ at those few initial nodes.

$$\left( \frac{h}{c\Delta t} \right)^2 \sin^2 \left( \frac{\omega \Delta t}{2} \right) = \tilde{p}_x^2 + \tilde{p}_y^2 + \tilde{p}_z^2 =$$
Figure 2.10: Left: Scattered Field $E_x$ (on Z planes) for which part of the H-plane fall in total field region. Respective incident $H$ fields need to be subtracted from these $H$ fields. Right: Scattered Field $E_x$ (on X planes) for which part of the H-plane fall in total field region. Respective incident $H_z$ fields need to be subtracted from these $H$ fields. Also included are some special cases at the corners.

Figure 2.11: Scattered Field $E_x$ (diagonally outside the TF along the Y axis) for which part of the H-plane fall in total field region. Respective incident $H$ fields need to be subtracted from these $H$ fields.

\[
\left\{ K_a \sin \left( \frac{k_x h}{2} \right) + \frac{1}{3} \sin \left( \frac{k_x h}{2} \right) \cdot \left[ K_b + \frac{K_c}{2} (\cos (\tilde{k_y} h) + \cos (\tilde{k_z} h)) + K_d \cos (\tilde{k_y} h) \cos (\tilde{k_z} h) \right] \right\}^2
\]
+ \left\{ K_a \sin (\tilde{k}_y h/2) + \frac{1}{3} \sin (\tilde{k}_y h/2) \cdot \left[ K_b + \frac{K_c}{2} \left( \cos (\tilde{k}_z h) + \cos (\tilde{k}_z h) \right) + K_d \cos (\tilde{k}_z h) \cos (\tilde{k}_z h) \right] \right\}^2 \\
+ \left\{ K_a \sin (\tilde{k}_z h/2) + \frac{1}{3} \sin (\tilde{k}_z h/2) \cdot \left[ K_b + \frac{K_c}{2} \left( \cos (\tilde{k}_x h) + \cos (\tilde{k}_y h) \right) + K_d \cos (\tilde{k}_x h) \cos (\tilde{k}_y h) \right] \right\}^2 \\
(2.7)

The first method is similar to the incident field array (IFA) method \[38\], however, the necessity for interpolation doesn’t arise because every location on the 3D grid has an equivalent point on the 1D grid. Having solved for the numerical $\tilde{k}$ at the center frequency of the pulse, the approximate time series (time waveform) at any further nodes can be found by applying spatial phase delay to the waveform $f(n)$ at reference location as shown in equation \[2.8\]. $\eta$ is the impedance of the homogeneous medium. Considering a modulated Gaussian pulse, $f(n)|_{ref} = e^{j\omega_0(n\Delta t - n_0)}e^{-\frac{n\Delta t - n_0}{n_0}}$, in a dispersive medium (such as an FV24 grid), the envelop travels with the group velocity, where as the carrier propagates with its phase velocity assuming the approximation $\tilde{k}(\omega) = \tilde{k}_0 + \tilde{k}_0' (\omega - \omega_0)$ is valid. Here, $\omega_0/\tilde{k}_0$ is the phase velocity of the carrier and $1/\tilde{k}_0'$ is the group velocity (at carrier frequency $\omega_0$) of the envelope.

\begin{align*}
  f_E(n)|_{i_r - 1/2} &= \text{Re}\{ f(n)|_{ref} \cdot e^{-j\tilde{k}_0(i_r - \frac{1}{2})\Delta r} \}, \\
  f_H(n - 1/2)|_{i_r} &= \frac{1}{\eta} \text{Re}\{ f(n - 1/2)|_{ref} \cdot e^{-j\tilde{k}_0 i_r \Delta r} \} \\
(2.8)
\end{align*}

The implementation given in equation \[2.8\] is overly simplistic as it delays only the carrier and neglects the group velocity. It considers the wavenumber at every frequency in the pulse to be same and equal to the wave number of the carrier. This causes distortion of the pulse at the point where the transition happens on the 1D grid from hard-wired part to the 1D update equation. One would need to delay the envelope considering the group velocity to reduce this distortion. Moreover, it is observed that the numerical wave number in the FV24 grid closely follows the free-space wave number for a sufficiently band limited pulse, so we can approximate the group velocity as equal to the phase velocity of the carrier. This formulation is given in equation \[2.9\].

\begin{align*}
  f_E(n)|_{i_r - 1/2} &= \cos \left( \omega_0[n\Delta t - n_0] - \tilde{k}_0[i_r - \frac{1}{2}]\Delta r \right) \cdot e^{-\frac{n\Delta t - n_0 - \tilde{k}_0[i_r - \frac{1}{2}]\Delta r}{n_0}} \cdot e^{-\frac{n\Delta t - n_0 - \tilde{k}_0[i_r - \frac{1}{2}]\Delta r}{n_0}} \cdot e^{-\frac{n\Delta t - n_0 - \tilde{k}_0[i_r - \frac{1}{2}]\Delta r}{n_0}} \\
  f_H(n - 1/2)|_{i_r} &= \cos \left( \omega_0[(n - 1/2)\Delta t - n_0] - \tilde{k}_0[i_r \Delta r] \right) \cdot e^{-\frac{(n - 1/2)\Delta t - n_0 - \tilde{k}_0[i_r \Delta r]}{n_0}} \cdot e^{-\frac{(n - 1/2)\Delta t - n_0 - \tilde{k}_0[i_r \Delta r]}{n_0}} \\
(2.9)
\end{align*}
Ideally, the numerical wave number should be solved for at every frequency in the pulse, multiply $e^{-j\tilde{k}(\omega)t_i\Delta r}$ with the Fourier transform of the time series at the reference point, then apply the inverse Fourier transform to get time series at locations that fall $i_r\Delta r$ units beyond the reference point on the 1D grid. This method was initially applied to the the 3D grid and called the Analytic Field Propagator (AFP) [39], and later adapted to the 1D grid by Tan and Potter as Optimized AFP (O-AFP). As we need fields only at few initial points using this method, a single phase velocity (of the most energetic frequency component, the carrier) is used. The formulation is given in equation 2.10. For a discussion on choice of number of points in FFT and inverse FFT, one can refer to [21,39].

\[
E_x(n)|_{i_r-1/2} = \text{Re}\{\text{FFT}^{-1}\left(\text{FFT}\left[\text{Re}\{F(n)|_{ref}\}\right]\right) \cdot e^{-j\tilde{k}_0(i_r-\frac{1}{2})\Delta r}}\},
\]

\[
H_x(n-1/2)|_{i_r} = \frac{1}{\eta} \text{Re}\{\text{FFT}^{-1}\left(\text{FFT}\left[\text{Re}\{F(n-1/2)|_{ref}\}\right]\right) \cdot e^{-j\tilde{k_0}i_r\Delta r}}\} \tag{2.10}
\]

For both the methods, once we have the time series for electric and magnetic fields, respective components ($E_{x,y,z}$ and $H_{x,y,z}$) can be expressed using the polarization projections in equations 2.12. Here, $\psi$ is the angle the vector $E$ makes with $\hat{z} \times \hat{P}$ and it is assumed to be known [12]. Those parameters with $\tilde{}$ represent numerical counterparts of continuous world. The FV24 numerical angels can be calculated using equations 2.11 as given in [21], where $\tilde{p}_{x,y,z}^2$ are obtained from the right hand side of equation 2.7 after solving for $\tilde{k}$.

\[
\tan \tilde{\phi} = \frac{\tilde{p}_y}{\tilde{p}_x}, \quad \tan^2 \tilde{\theta} = \frac{\tilde{p}_x^2 + \tilde{p}_y^2}{\tilde{p}_z^2} \tag{2.11}
\]

\[
E_x|_{i_r-1/2} = f_{E(n)}|_{i_r,1/2} \cdot (\cos \psi \sin \tilde{\phi} - \sin \psi \cos \tilde{\theta} \cos \tilde{\phi})
\]

\[
E_y|_{i_r-1/2} = f_{E(n)}|_{i_r,1/2} \cdot (\cos \psi \cos \tilde{\phi} - \sin \psi \cos \tilde{\theta} \sin \tilde{\phi})
\]

\[
E_z|_{i_r-1/2} = f_{E(n)}|_{i_r,1/2} \cdot (\sin \psi \sin \tilde{\theta})
\]

\[
H_x|_{i_r} = f_{H(n)}|_{i_r} \cdot (\sin \psi \sin \tilde{\phi} + \cos \psi \cos \tilde{\theta} \cos \tilde{\phi})
\]

\[
H_y|_{i_r} = f_{H(n)}|_{i_r} \cdot (\cos \psi \cos \tilde{\phi} + \cos \psi \cos \tilde{\theta} \sin \tilde{\phi})
\]

\[
H_z|_{i_r} = f_{H(n)}|_{i_r} \cdot (\cos \psi \sin \tilde{\theta}) \tag{2.12}
\]
The number of initial nodes that are hard wired for each component is selected based on avoiding the negative indexes that may arise in the 1D update equations. Also, a common number of hard wired nodes for all field components will not work because the first $E_{x,y,z}$ nodes that should be updated on the 1D grid are not co-located. To see this subtlety, consider that the corner of the TF region to be $(x, y, z)$ and its projection on the 1D grid to be $m_0 \Delta r$. At any time step, the location of the first $E_x$ (of the TF region) on the 3D grid is $(x + \frac{h}{2}, y, z)$ whose projection and index on the 1D grid are $(m_0 + \frac{m_x+1}{2})\Delta r$ and $m_0 + \frac{m_x+1}{2}$ respectively. For $E_y$, they are $(m_0 + \frac{m_y+1}{2})\Delta r$ and $m_0 + \frac{m_y+1}{2}$. Similarly index is $m_0 + \frac{m_y+1}{2}$ for $E_z$, $m_0 + \frac{m_x+m_z}{2}$, $m_0 + \frac{m_y+m_z}{2}$, and $m_0 + \frac{m_x+m_y}{2}$ for $H_{x,y,z}$ respectively. Observing that they are offset by different amounts from $m_0$, the field component updates on the 1D grid should start in the same staggered manner. Otherwise, the time and space offsets inherent to any FDTD scheme are not taken care of and wrong field values from right locations are picked up on the right hand side of the update equations by the algorithm. Therefore, the hard wiring is done up to index $m_0 + \frac{m_x+1}{2} - 1$, $m_0 + \frac{m_y+1}{2} - 1$, $m_0 + \frac{m_z+1}{2} - 1$ and $m_0 + \frac{m_x+m_z}{2} - 1$, $m_0 + \frac{m_x+m_z}{2} - 1$, and $m_0 + \frac{m_x+m_y}{2} - 1$ for $E_{x,y,x}$ and $H_{x,y,z}$ respectively.

2.3 Validations of the Injection Technique

The above TF/SF method for exciting a plane wave in an FV24 grid is implemented with no scatterers inside the TF region for the sake of demonstration. As we would expect to see no signal in the SF region in the absence of scatterers, the lattice truncation using PML or CPML is not necessary to implement, however, their inclusion is straight forward. The wave form initiated on the 1D and so on 3D grid is a modulated Gaussian pulse $f(n)|_{ref} = e^{j\omega_0(n\Delta t-n_0)}e^{-\frac{(n\Delta t-n_0)^2}{n_\sigma}}$ where $n_0$ and $n_\sigma$ (despite $n$ in their name, $n_0$ and $n_\sigma$ have units of time) are used to vary the bandwidth and the time shift of the Gaussian pulse. $n_0$ should be selected such that the pulse rises gradually from zero. If $n_0$ is not sufficiently large, the time series $Re(f(n))$ will start abruptly in time and also in space (on the 1D grid near the transition from hard sourcing to take over by 1D update equations). This results in distortion of the waveform on 1D grid because of the high frequency components associated with an abrupt change.
The choice of $n_\sigma$ decides the width of the pulse in time and frequency domain, the larger the value the broader is the pulse in time domain and narrower in frequency domain. Smaller $n_\sigma$ will increase the highest frequency component in the pulse which may distort the pulse as it propagates on the 1D grid (manifests itself on the 3D grid as well) because of insufficient grid resolution and resultant FV24 numerical dispersion. However, pulse distortion because of too small $n_0$ and/or $n_\sigma$ will not effect the field leakage in to the SF region as long as the TF/SF corrections are done properly. For a distortion free pulse propagation, we chose $n_\sigma = \frac{2\sqrt{\frac{3}{2}}}{\pi \Delta f}$ and $n_0 = 4.5n_\sigma$ as recommended in [1]. Here $\Delta f$ is the range of frequencies of the Gaussian pulse spectrum around carrier frequency with a amplitude of 10% of the maximum or more.

The simulations are carried out with a carrier frequency of $f_0 = 2$ GHz, uniform grid resolution of 20 cells per wavelength at 1 GHz, and $\Delta t = \frac{\hbar}{c \sqrt{3} \left| 3 - 4K_b - 2K_c - 4K_d \right|}$ (the upper limit provided in [23]). The TF region size is 40X40X40, and the SF region extends 10 cells from the TF region in every direction. The integers $(m_x, m_y, m_z) = (9, 3, 13)$ and the polarization angle $\psi = \pi/2$. With hard sourcing similar to IFA (first of the two methods described above), the wave forms for $E_x$ and $H_z$ after propagating for 300 time steps on the 1D grid are shown in figure 2.12. The incident fields $E_x$ and $H_z$ in TF region at a Z plane cross-section are shown in figure 2.13.

Also, the leakage field for $E_x$ and $H_z$ at the same Z plane are shown in figure 2.14 after 300 time steps. As expected, the leakage for all the field components is -300 dB below the respective incident field strengths.

### 2.4 Comparison of Near-to-Farfield Transformation Techniques for FDTD

Equivalence theorems in EM come very handy to efficiently calculate/project farfields from a radiating source or a scatterer. Extending the problem space to include the farfield region is not often computationally feasible due to time and memory costs involved. Equivalence theorems stipulate that farfield radiation or scattering profile (of a source or scatterer) can be evaluated from the nearfields. The nearfields in the form of fictitious electric and magnetic surface currents ($J_s$ and $M_s$) are chosen on an equivalent surface enclosing the source or the scatterer. The surface
currents on the equivalent surface are used to calculate the farfield vector potentials \( \mathbf{A} \) and \( \mathbf{F} \). These vector potentials are then used to obtain either radiation pattern in case of sources or radar cross section (RCS) in case of scatterers. The surface currents, \( J_s \) and \( M_s \), are in turn calculated from nearfield tangential magnetic and electric fields (to the equivalent surface), respectively. This process is referred to as near-to-farfield transformation.

Near-to-Farfield transformation in FDTD has been applied to satisfactorily predict the farfield radiation/scattering profiles. One peculiar thing about constructing equivalent surface in FDTD is that, it is not possible for any single closed surface to house both the tangential electric \( E \) and magnetic \( H \) nearfields (that are used to calculate surface currents \( J_s \) and \( M_s \)). The reason being, the \( E \) and \( H \) fields are not co-located in the FDTD grid (staggered in space). This makes it
necessary to interpolate fields from neighboring Yee cells in order to bring $E$ and $H$ (and thereby $J_s$ and $M_s$) onto the same surface.

Different interpolation schemes available in the literature are arithmetic averaging [1], geometric mean [41] and the mixed-surface approach [42]. In this work, we compare FDTD farfield profiles of a empty scattering region, for which farfields should be ideally zero. The farfields are obtained from surface currents calculated using different interpolation techniques mentioned above, and also a separate surface approach dealt later in this chapter.

The equivalent surface, on which near-to-farfield transformation is performed, is placed in the scattered field region as shown in figure 2.13. The scattered fields on this equivalent surface are used to calculate surface currents, which are used in the surface integrals to calculate vector potentials.

However, as mentioned earlier, in FDTD a single equivalent surface will not house both the
Figure 2.14: Top: Leakage of $E_x$ into SF on a Z plane at the center of TF after 300 time-steps. Bottom: Leakage of $H_z$ into SF on a Z plane at the center of TF after 300 time-steps.

Figure 2.15: Schematic of the FDTD problem space, showing the dielectric scatterer, TF/SF regions and the Equivalent surface.

tangential magnetic and electric fields (or surface currents), because of the staggered field locations in FDTD grid, as shown in figure 2.16.
2.4.1 Arithmetic and Geometric Averaging

One of the techniques to bring the surface currents ($J_s$ and $M_s$) on to the same surface is to interpolate electric and magnetic fields using arithmetic average. Average of four H fields and two E fields (time-domain fields) brings currents onto the same surface and to the same location, as demonstrated in [1]. This is shown in figure 2.17. Discrete Fourier Transform (DFT) is applied on the time-domain average to obtain frequency-domain current components, at the desired frequencies. These frequency-domain currents are obtained at discrete locations, covering all the six faces of the equivalent surface.

The geometric-mean interpolation is performed on the same fields as used by arithmetic averaging, shown in figure 2.17. However, a different sequence of steps is followed. First, the DFT is applied on the four time-domain H fields and the two time-domain E fields at the desired frequencies, then the geometric mean of the complex-valued frequency-domain currents are obtained at all the discrete locations of the equivalent surface. Directly applying geometric mean on time-domain fields would force us take the square root and fourth root of negative real values. First applying DFT and then taking the geometric mean would help avoid this. While applying geometric mean on complex values, care should be taken to convert (wrap) the angle of complex values from...
Figure 2.17: Left: Average of two Electric field components highlighted red. Right: Average of four Magnetic field components highlighted red.

$[-\pi, \pi]$ scale to $[0, 2\pi]$ scale. This allows the complex geometric mean to bisect the angle between the two/four complex operands.

### 2.4.2 The Separate and Mixed Surface Approach

Another technique to overcome staggered-nature of planes containing tangential currents in FDTD, for performing near-to-farfield transformation, is mixed-surface approach introduced in [42]. Similarities exist between mixed-surface approach and TF/SF formulation. For example, the fictitious surface currents introduced at the TF/SF interface in the TF/SF formulation, in the form of consistency corrections to the FDTD update equations, where they excite equivalent planewave fields inside the total field region, required no interpolation. This mixed-surface approach is counterpart (dual) to the TF/SF formulation, in the sense that it also does not use field interpolation to launch equivalent farfields outside the equivalent surface.

During the consistency corrections to the electric field in TF/SF formulation, for example, we add or subtract incident magnetic field to the right hand side of the update equation. This is analogous to placing a magnetic field-generated electric surface current at the electric field location, i.e., shifting the location of electric surface current from the location of its associated magnetic field. Similarly, the location of magnetic surface current is changed from the location of its asso-
ciated electric field. This mixing of field and current locations, when applied to near-to-farfield transformation, is referred to as the Mixed-Surface approach \[42\].

The implementations of the mixed-surface approach is shown in equations \[2.13\] and figure \[2.18\]. \(S_e\) and \(S_h\) represent two surfaces on which the tangential electric and magnetic fields are present, respectively, in FDTD grid. When evaluating the surface integral for \(N\) in equations \[2.13\] using the magnetic fields on \(S_h\), the surface electric currents caused by the magnetic fields \((\mathbf{J}_s = \hat{n} \times \mathbf{H})\) are assumed to be placed on \(S_e\). Therefore, the distance (between the reference point, i.e. the center of the volume enclosed by equivalent surface, and the current location on \(S_e\)) \(r_e'\) is used in the exponential inside the integral.

Similarly, when evaluating the surface integral for \(L\) in equations \[2.13\] using the electric fields on \(S_e\), the surface magnetic currents caused by the electric fields \((\mathbf{M}_s = -\hat{n} \times \mathbf{E})\) are assumed to be placed on \(S_h\). Thus, the distance \(r_h'\) is used in the exponential term inside integral.

\[
\begin{align*}
N &= \iint_{S_h} \hat{n} \times \mathbf{H} |_{S_h} e^{jk \cdot r_e'} dS' = \iint_{S_h} \mathbf{J}_s |_{S_e} e^{jk \cdot r_e'} dS' \\
L &= -\iint_{S_e} \hat{n} \times \mathbf{E} |_{S_e} e^{jk \cdot r_h'} dS' = \iint_{S_e} \mathbf{M}_s |_{S_h} e^{jk \cdot r_h'} dS' 
\end{align*}
\tag{2.13}
\]

Figure 2.18: Left: Magnetic field-produced electric currents are placed on \(S_e\). Right: Electric field-produced magnetic currents are placed on \(S_h\)

Finally, a separate-surface approach, which does not involve any mixing of field and current
location and similar to mixed-surface approach in all other aspects, is implemented.

2.5 Frequency Domain Near-to-Farfield Transformation in FDTD

The frequency domain near-to-farfield projection is defined in terms of vector potential functions \( \mathbf{A} \) and \( \mathbf{F} \) in equations 2.14. They are functions of frequency and farfield position unit vector \( \hat{\mathbf{r}} \) along \( \mathbf{r} \) as shown in figure 2.15. The unit vector also represents farfield angles \( \theta \) and \( \phi \). The closed surface integral is over the equivalent surface. The frequency domain currents \( \mathbf{J}_s \) and \( \mathbf{M}_s \) (complex-valued) are functions of position on the equivalent surface (represented by primed position vector \( \mathbf{r}' \) as shown in figure 2.15) and the frequency.

\[
\begin{align*}
\mathbf{A}(\hat{\mathbf{r}}, \omega) &= \frac{\mu_0 e^{-jkR}}{4\pi R} \iint_S \mathbf{J}_s(\mathbf{r}', \omega) e^{jk\hat{\mathbf{r}} \cdot \mathbf{r}'} dS' = \frac{\mu_0 e^{-jkR}}{4\pi R} \mathbf{N}, \\
\mathbf{F}(\hat{\mathbf{r}}, \omega) &= \frac{\varepsilon_0 e^{-jkR}}{4\pi R} \iint_S \mathbf{M}_s(\mathbf{r}', \omega) e^{jk\hat{\mathbf{r}} \cdot \mathbf{r}'} dS' = \frac{\varepsilon_0 e^{-jkR}}{4\pi R} \mathbf{L}
\end{align*}
\]  

(2.14)

The auxiliary vectors \( \mathbf{N} \) and \( \mathbf{L} \) in equations 2.14 that represent only the surface integrals, are then used to calculate the \( \theta \) and \( \phi \) components of farfield Electric field, given by equations 2.15.

\[
\begin{align*}
E_\theta(\theta, \phi, \omega) &= -\frac{j\varepsilon_0 e^{-jkR}}{4\pi R} (L_\phi + \eta_0 N_\theta), \\
E_\phi(\theta, \phi, \omega) &= \frac{j\varepsilon_0 e^{-jkR}}{4\pi R} (L_\theta - \eta_0 N_\phi)
\end{align*}
\]  

(2.15)

where \( k \) and \( \eta_0 \) are the free-space wave-number and the intrinsic impedance, respectively. The surface integration in equations 2.14 are carried as discrete summations (Riemann Sum). And, \( P_{inc} \) is the power density of the incident planewave, given by \( P_{inc} = \frac{1}{2\eta}(E_\theta^2 + E_\phi^2) \cdot |F(\omega)|^2 \), where \( F(\omega) \) is the Fourier transform of time-series \( f(t) \) which is defined in equations 2.18 sampled at the desired frequency \( \omega \).

The \( \theta \) and \( \phi \) components of the auxiliary vectors \( \mathbf{N} \) and \( \mathbf{L} \) are defined by equations 2.16 as
given in [1].

\[ N_\theta = \oint_S \left( J_x \cos(\theta) \sin(\phi) + J_y \cos(\theta) \sin(\phi) - J_z \sin(\theta) \right) e^{jkr'\cos(\psi)} dS', \]

\[ N_\phi = \oint_S \left( - J_x \sin(\phi) + J_y \cos(\phi) \right) e^{jkr'\cos(\psi)} dS', \]

\[ L_\theta = \oint_S \left( M_x \cos(\theta) \sin(\phi) + M_y \cos(\theta) \sin(\phi) - M_z \sin(\theta) \right) e^{jkr'\cos(\psi)} dS', \]

\[ L_\phi = \oint_S \left( - M_x \sin(\phi) + M_y \cos(\phi) \right) e^{jkr'\cos(\psi)} dS'. \]

(2.16)

2.6 Error Comparison with a No Scatterer

As a way to benchmark the accuracy of the above interpolation schemes, an empty region (no-scatterer) is illuminated by a plane wave using Discrete Planewave technique with TF/SF formulation described earlier in the chapter. Then, the farfields are obtained from the nearfields which are interpolated using different schemes dealt with in the previous section, and compared. As one might expect, the no-scatterer case should ideally result in zero farfield. Any farfield electric field in equation 2.15 observed is an error (the noise floor). Errors can be because of:

- Numerical Dispersion
- \( J_s \) and \( M_s \) calculation
- Surface integration
- Discretization in space and time
- Truncation (Finite word length)

Although this work doesn’t attempt to separate the above, the error in farfield caused by the miscalculation (interpolation) of \( J_s \) and \( M_s \) is the main differentiator. This is because, all the other error contributors itemized above are identical for all the interpolation techniques. Therefore, it is expected that the interpolation scheme that gives minimum farfield performs better than the rest in terms of accuracy.
The above interpolations schemes are compared for three different simulation parameters:

1. Resolution of the FDTD grid,
2. Incident angle of the plane wave,
3. Size of the equivalent surface.

### 2.6.1 Resolution Sweep

Figure 2.19 shows how different interpolation schemes compare for different resolution of the grid. The vertical axis is the maximum of $E_\theta \cdot \Delta t$ or $E_\phi \cdot \Delta t$ in dB, observed in all the farfield principal planes (XY, XZ, and YZ planes). Here $\Delta t$ is the FDTD discretization time step. The horizontal axis is the grid resolution in terms of cells per wavelength. The frequency at which the farfields are calculated is 2 GHz.

![Figure 2.19: Maximum farfield error in dB for different grid resolutions.](image)

On the other hand, figure 2.20 shows average of $E_\theta \cdot \Delta t$ and $E_\phi \cdot \Delta t$ observed in all the farfield principal planes.

The incident angle for the plane wave is $\phi_{inc} = 35.5^0, \theta_{inc} = 38^0$ and the size of equivalent surface is $(1\lambda)^3$. As expected, the farfield error decreases as resolution increases because the discretization errors in FDTD get minimized as the grid gets finer and finer.
2.6.2 Incident Angle Sweep

Figures 2.21, 2.22 shows how maximum and average errors compare for different interpolation schemes at different incident angles of the plane wave. The vertical axis is same as described before and the horizontal axis specifies the $\theta_{inc}$ direction of the plane wave while the $\phi_{inc} = 23.2^\circ$. The size of the equivalent surface is $(5\lambda)^3$ and the grid resolution is 10 cells per wavelength. The frequency at which the farfields are calculated is 2 GHz.

The trend suggests that as incident plane wave direction gets close to the axes directions ($\theta_{inc} = 0, 90^\circ$), the farfield errors increase. This might be because of FDTD numerical dispersion errors becoming worse for waves propagating along the axes directions as demonstrated in [12].
2.6.3 Equivalent Surface Size Sweep

Figures 2.23, 2.24 shows how maximum and average errors compare for different interpolation schemes for different equivalent surface sizes. The vertical axis is same as described before and the horizontal axis specifies the size of equivalent surface as multiple of $\lambda$ in $6(n\lambda)^2$. The incident angle for the plane wave is $\phi_{inc} = 35.5^0, \theta_{inc} = 38^0$ and the grid resolution is 10 cells per wavelength. The frequency at which the farfields are calculated is 2 GHz. As expected, the farfield errors increase as size of equivalent surface increases. This is because, the phase errors in FDTD accumulate more as the wave travels in the grid longer and longer.

The comparison suggests that the mixed surface and arithmetic mean interpolation schemes perform consistently better when compared to the geometric mean interpolation and separate surface approach.

Figure 2.23: Maximum farfield error in dB for various equivalent surface sizes.
2.6.4 Bistatic RCS Comparison for a Dielectric Cube

To further validate the performance of different FDTD interpolation schemes, the bistatic RCS of a dielectric cube ($\epsilon_r = 5, \mu_r = 1$) is calculated at a single frequency of 1 GHz. This FDTD farfield scattering profile is compared with those obtained from integral equation solvers available in FEKO and HFSS.

The auxiliary vectors $N$ and $L$ in equations 2.14 that represent only the surface integrals, are used to calculate the $\theta$ and $\phi$ components of RCS, given by equations 2.17:

$$RCS_\theta(\theta, \phi, \omega) = \frac{k^2}{8\pi\eta_0 P_{inc}} |L_\phi + \eta_0 N_\theta|^2,$$

$$RCS_\phi(\theta, \phi, \omega) = \frac{k^2}{8\pi\eta_0 P_{inc}} |L_\theta - \eta_0 N_\phi|^2,$$  \hspace{1cm} (2.17)

The polarization of the planewave is defined by $E_\phi$ and $E_\theta$, same as how planewave polarization is defined in HFSS and is similar to FEKO’s definition. In FEKO, the planewave polarization is defined, slightly different, as the angle ($\eta$) Electric field vector makes with $-\hat{\theta}$ (unit vector at planewave arriving angles). As an example of an identical setup in the three solvers, choosing the angle $\eta$ as $180^0$ in FEKO and $E_\theta = 1 \& E_\phi = 0$ in FDTD and HFSS for the planewave will make it theta-polarized. The polarization coefficients of the electric and magnetic fields in the X, Y and
Z directions are given by equations (2.18) as given in [1].

\[ E_{\text{inc},x} = [E_\theta \cos(\tilde{\theta}_{\text{inc}}) \cos(\tilde{\phi}_{\text{inc}}) - E_\phi \sin(\tilde{\phi}_{\text{inc}})] f(t), \]
\[ E_{\text{inc},y} = [E_\theta \cos(\tilde{\theta}_{\text{inc}}) \sin(\tilde{\phi}_{\text{inc}}) + E_\phi \cos(\tilde{\phi}_{\text{inc}})] f(t), \]
\[ E_{\text{inc},z} = -E_\theta \sin(\tilde{\theta}_{\text{inc}}) f(t), \]
\[ H_{\text{inc},x} = -\frac{1}{\eta_0} [E_\phi \cos(\tilde{\theta}_{\text{inc}}) \cos(\tilde{\phi}_{\text{inc}}) + E_\theta \sin(\tilde{\phi}_{\text{inc}})] f(t), \]
\[ H_{\text{inc},y} = -\frac{1}{\eta_0} [E_\phi \cos(\tilde{\theta}_{\text{inc}}) \sin(\tilde{\phi}_{\text{inc}}) - E_\theta \cos(\tilde{\phi}_{\text{inc}})] f(t), \]
\[ H_{\text{inc},z} = \frac{1}{\eta_0} E_\phi \sin(\tilde{\theta}_{\text{inc}}) f(t) \quad (2.18) \]

The dielectric cube of size \( \lambda/2 \) on each side (at 1 GHz) is illuminated with a plane wave incident at \( \theta_{\text{inc}} = 38.0^0 \) and \( \phi_{\text{inc}} = 35.5^0 \). This incident angle is rendered by the choice of integers \((m_x,m_y,m_z)\) as \((7,5,11)\) in the perfect TF/SF formulation described in the initial sections of the chapter. These angles in FDTD indicate the direction of planewave propagation (direction of propagation vector). Contrary to this, HFSS and FEKO would require the direction the planewave comes from (opposite to the direction of propagation vector). Consequently, the planewave arrival angles, \( \theta_{\text{arrival}} = 180 - \theta_{\text{inc}} \) and \( \phi_{\text{arrival}} = 180 + \phi_{\text{inc}} \), are used in these solvers. The time-profile of the theta-polarized planewave is a modulated Gaussian pulse, with frequency spectrum centered around 1 GHz.

The RCS results from the four interpolation schemes of interest –arithmetic averaging, geometric mean, mixed-surface, separate-surface approach– are compared with RCS profiles obtained from FEKO-MoM and HFSS-IE in figures 2.25.

These figures show clear advantage that the mixed surface and arithmetic averaging schemes have over the other two, geometric mean and separate surface approach. Here, the FDTD grid resolution used is 40 cells/wavelength at 1 GHz. Here, only \( RCS_\theta \) comparison is shown on the three farfield cuts (principal planes) as the \( RCS_\phi \) results do not deviate from each other to a perceivable degree.
Figure 2.25: The \( \theta \) component of bistatic RCS in different farfield planes. FDTD resolution is 40 cells/wavelength at 1 GHz.
Chapter 3

Analysis of Glass Weave Induced Skew in Differential Pairs

This chapter deals with the timing skew between the two signals on a differential pair because of glass fiber weave inside the PCB composite. As the interconnects on a high-speed printed circuit boards carry more bits per second, skew becomes more crucial to predict and control. Accurate simulation models to estimate the glass-weave skew and thereby predict the bit error rate, and the differential-to-common signal conversion are very helpful in the robust design of high-speed boards.

Finite difference time domain (FDTD) technique with its inherent capability to produce transient (time-domain) and wide-band (frequency-domain) responses might better suit this skew study. The challenges in FDTD are to implement frequency-dependent dielectric losses (dispersive complex permittivity) with high degree of accuracy.

This work demonstrates that FDTD, with the help of the techniques available in the literature, can successfully estimate the signal skew in high-speed PCBs. Skew can be extracted directly from the FDTD time-domain responses without the need for impulse responses constructed by inverse Fourier transforming S-parameters. Also, the FDTD simulation data in the form of S-parameters are bench-marked with frequency-domain finite element solver in HFSS. It also demonstrates that the acceleration of FDTD using the GPU in MATLAB leads to faster FDTD simulations.

3.1 Introduction: Glass Weave Skew in High Speed PCBs

Modern printed circuit boards (PCB) contain many dielectric (core and prepeg) and metallic layers stacked on top of each other as shown in figure 3.1. The dielectric layer is a composite
material having woven glass fiber and resin (epoxy). The resin binds the glass fiber and hence aptly called binder. The binder material is also referred to as the matrix \[43\]. Core is a cured dielectric available to PCB manufacturers with copper cladding on both sides, whereas prepreg is a uncured dielectric and acts as a glue when all the layers are pressed together to form a PCB \[3\].

![Figure 3.1: Stack-up of a fourteen layer PCB \[3\], as an example.](image)

Glass fiber weave is available in many different styles as shown in figure \[3.1\] \[44\], and appropriate selection of glass style is important in mitigating glass weave induced skew (discussed later) and for a robust current high-speed PCB designs.

![Figure 3.2: Different glass weave styles and their style numbers.](image)

Figure \[3.3\] shows a CAD model of the woven glass fiber and resin composite material. As
shown in the figure, dielectric layer is an in-homogeneous material of glass and resin with glass-rich and resin-rich areas. Moreover, these two materials, glass and resin, have inherently different electrical properties. Comparatively, glass is a high permittivity, low loss material while resin is a low permittivity, high loss material. This results in the microscopic variation of material properties. Therefore, the electrical properties of copper traces (microstrip or striplines for example) etched on such a material vary with position depending whether they see more glass or more resin. For example the microstrip trace shown in figure 3.3 falls entirely on glass fiber and so sees more glass. That means the propagation delay of two conductive traces might vary even though they have same physical properties and are parallel to each other.

Figure 3.3: A CAD model showing woven glass fiber and resin composite material. Also shown are glass-rich and resin-rich areas and a microstrip trace

In todays high speed PCBs, the differential signaling is widely used because of its immunity to cross talk, ground bounce, simultaneous switching noise, and less radiated emissions when compared to single-ended signaling [45], [46]. In differential signaling scheme on PCBs, a pair of conductive traces (Differential Pair) carry balanced signals that are out of phase (180 degrees phase difference). The two signals in the differential signaling should ideally be out of phase by 180 degrees at transmitter side and receiver side, canceling each other when added. However, because of asymmetries in the drivers, terminations, and in the channel (interconnects), there is certain imbalance between the two signals on the differential pair. The imbalance in time delay or propagation
delay between the two traces is often referred to as skew.

When the skew is imparted because of one trace 'seeing' more glass (or resin) than the other trace, i.e., because of difference in dielectric properties of glass fiber and resin, it is referred to as Glass Weave skew (GWS). The signal on the trace that sees more glass will propagate slower than the signal on the trace that sees more resin. This effect is called Fiber Weave Effect (FWE). As shown in figure 3.4 Trace 1 in the differential pair falls on glass fiber, i.e., in the glass-rich region, whereas the Trace 2 falls in between glass fibers, i.e., in the resin-rich region. The effective dielectric constant seen by the former is more than that of what is seen by the latter. This results in signal on it traveling slower than the signal on the other trace, giving rise to glass weave induced skew. In today’s high bandwidth networking devices (switches and routing platforms), where digital signals pass through traces tens of inches long, the skew can accumulate to several pico-seconds.

![Figure 3.4](image)

Figure 3.4: A model showing two traces of a microstrip differential pair, one that falls entirely on glass fiber bundle and one that glass in between glass fiber bundles.

The skew results in a non-zero average of the two signals at the receiver end, i.e., results in a common signal on the differential pair. This common signal, sometimes referred to as common-mode signal, can severely effect the integrity of the signal at the receiver. For example, it causes resonances in the $SDD_{21}$ which is the differential insertion loss, leading to closure of eye diagrams and increasing bit error rates. It might also cause unintended radiation resulting in electromagnetic
compatibility (EMC) issues.

3.1.1 FDTD Modeling of Glass-Resin Composites: Motivation

The estimation of skew can be helpful to the system designers to see if the worst case skew is within tolerable levels, even before they start thinking about mitigation techniques. Full wave 3D field solvers can estimate the skew for ideal PCB board designs. Although, the real PCB boards are bound to have some manufacturing defects/variations, a reliable estimate of skew is expected from the 3D field solvers to aid system designers. Commercial frequency domain solvers such as HFSS, can be used to obtain S-parameters (scattering parameters) over a range of frequencies the board operates in. These S-parameters are in turn used to construct time domain pulse (with non-zero rise time) response of individual traces in the differential pair. Finally, comparing the two pulses gives an estimate of skew. Inverse Fourier transform is invariably involved in this frequency domain to time-domain conversion.

The conversion of frequency domain S-parameters to get time-domain skew is expected to have certain errors. The choice of number of frequency points, the highest frequency for which data is available, and the input pulse rise-time during the inverse Fourier transform operation might lead to miscalculation of skew. Moreover, the need to solve for S-parameters accurately over a large number of discrete frequencies to get better resolution in time and thereby obtain accurate estimate of skew is the main disadvantage with frequency-domain solvers.

This disadvantage and the uncertainty in estimation of skew can be overcome by using finite difference time domain (FDTD) method. With its inherent ability to produce time domain responses, FDTD can estimate the glass weave skew with minimal post processing of EM fields. While the finite element solvers have the ability to model the inhomogeneities of the PCB more accurately because of the tetrahedral meshing, the simplest FDTD method uses rigid rectangular cuboid grid. This should have minimal impact as long as a finer mesh is used in FDTD. Using finer meshes increases the computational cost, a trade-off for accuracy. Given that the FDTD is easily and massively parallelizable, and with the cheap compute power available, the accuracy can
be maintained.

The differential trace pair shown above in figure 3.4 with a loss-less dielectric and conductor material properties as in table 3.1 is simulated using FDTD. The update equations, sourcing, probing and PML boundary implementation are as provided in [1]. The waveform at the source side of two traces is a Gaussian pulse having frequency components in excess of 40 GHz which is the typical bandwidth of today’s high-speed digital signals. Two probes (Probe 1 and 2) are placed on receiver side of Traces 1 and 2 in figure 3.4. Figure 3.5 shows the voltage waveforms sensed by probes 1 and 2. Implementing the loss less or flat-loss dielectric materials using in-house FDTD codes is straight-forward as given in [1].

Table 3.1: Loss-less Material Properties

<table>
<thead>
<tr>
<th>Material</th>
<th>Dielectric Constant ($\varepsilon_r$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resin Dielectric</td>
<td>3.2</td>
</tr>
<tr>
<td>Glass Dielectric</td>
<td>5.6</td>
</tr>
</tbody>
</table>

Figure 3.5: Voltage waveforms show slight glass-weave induced timing skew on a differential a pair.
3.1.2 Implementation of Glass Weave Structure in FDTD Grid

In the FDTD material grid, a glass weave fiber face is implemented mathematically as an ellipse in $x - y$ plane as given in equation 3.1 below:

$$\left(\frac{x - x_0}{a}\right)^2 + \left(\frac{y - y_0}{b}\right)^2 = 1,$$

(3.1)

where $a$ and $b$ are major and minor axes radii. This ellipse is centered around $(x_0, y_0)$.

The center of this ellipse can be swept along a sinusoidal path along the PCB lengthwise direction (along $z$ axis, for example) as shown in equation 3.2 below:

$$\left(\frac{x - x_0}{a}\right)^2 + \left(\frac{y - \sin(w_g \cdot z)}{b}\right)^2 = 1,$$

(3.2)

where $w_g$ is wiggle factor that denotes how frequent are the undulations along the $z$ direction.

It can be noticed that the $x$-coordinate of the ellipse’s center is kept constant while the $y$-coordinate of the ellipse’s center depends on the position along the $z$-axis. The above procedure is depicted in figure 3.6. This models a glass fiber bundle in the PCB’s dielectric layer. This fiber bundle is replicated multiple times along the woof as well as the warp directions as shown in the figure to form a weave-like material structure. The FDTD cells whose centers fall inside the ellipse are assigned dielectric constant of the glass. Comparatively, microstrip trace and resin material implementation is easy in Cartesian FDTD because of their rectangular or square shape that conforms well with Cartesian coordinate system. Figure 3.7 shows a two-dimensional cross section of FDTD grid that models a PCB, including the glass weave structure, resin, and copper traces. The ground plane is implemented as zero-thickness PEC boundary condition and is not shown.

3.2 Frequency Dependent Losses: Dispersive Medium

Loss-less materials are used for the simulation in the previous section. Similarly, flat-loss ($\sigma$ is constant across frequencies) materials can be implemented simply by including the conductivity $\sigma$ in the FDTD update equations. However, real-world materials are lossy, i.e., they have complex
Figure 3.6: Glass fiber face modeled as an ellipse in \(x - y\) plane as shown above and is swept along the \(z\)-axis modulating the \(y\)-coordinate of the center of the ellipse as shown below.

Figure 3.7: Various materials assigned to the cells in the FDTD grid modeling a PCB dielectric constant and these losses are frequency dependent. These materials are causal i.e., the real and imaginary parts of complex permittivity satisfy Kramers-Kronig relationship.

This frequency dependence is often modeled using Djordjevic-Sarkar model as in equation 3.4. Implementing the frequency dependent losses of a PCB material for time domain FDTD simulation is not as straight forward as it is for frequency domain simulations. The logarithmic
terms in Djordjevic-Sarkar model are even more complex to transform to time domain. On the other
hand, Debye (given in equation [3.3]) and Lorentz models [10], which have $\omega$ frequency dependence,
can be transformed to time domain and implemented relatively easy using Auxiliary Differential
Equation (ADE) method.

$$
\varepsilon_r = \varepsilon_\infty + \sum_k A_k (\varepsilon_s - \varepsilon_\infty) + \frac{\sigma_{DC}}{\omega \varepsilon_0} \frac{1}{1 + j\omega \tau_k} \quad (3.3)
$$

$$
\varepsilon_r = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)}{\ln \left( \frac{\omega_B}{\omega_A} \right) \ln \left( \frac{\omega_A + j\omega}{\omega_B + j\omega} \right)} + \frac{\sigma_{DC}}{\omega \varepsilon_0} \quad (3.4)
$$

where:

- $\varepsilon_r$: frequency dependent relative permittivity,
- $\varepsilon_s$: relative permittivity at DC,
- $\varepsilon_\infty$: relative permittivity in the optical frequency range,
- $A_k$: a dimension less Debye model coefficient,
- $\omega$: the angular frequency,
- $\tau_k$: inverse of relaxation frequency,
- $\sigma_{DC}$: the conductivity at DC,
- $\varepsilon_0$: free space permittivity,
- $\omega_A, \omega_B$: lower and upper angular transition frequencies, respectively.

### 3.2.1 Adapting Djordjevic-Sarkar Model to FDTD

The Djordjevic-Sarkar model is suitable for FR4-type materials used in PCBs [47]. The
advantage of this model is that the material properties can be calculated from minimum measured
data points. For example, $\varepsilon_r$ and $\tan \delta$ in table 3.2 for glass/resin dielectrics measured at 1 GHz
(Courtesy: Cisco Systems, Inc.) are used in conjunction with equation 3.4 to extrapolate complex
permittivity over wide frequency ranges. This method is used in frequency domain solvers such as
finite element method in HFSS for broadband simulation of PCB models.

As mentioned earlier, the logarithmic terms in this model are a bottle neck for its imple-
mentation in FDTD. A workaround is to first generate complex permittivity values from available
Table 3.2: Material properties of glass and resin at 1 GHz

<table>
<thead>
<tr>
<th>Material</th>
<th>Dielectric Constant ($\epsilon_r$)</th>
<th>Loss tangent (tan $\delta$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resin</td>
<td>3.65</td>
<td>0.02</td>
</tr>
<tr>
<td>Glass</td>
<td>6</td>
<td>0.0058</td>
</tr>
</tbody>
</table>

measured data by using Djordjevic-Sarkar model over a wide frequency range, then fit a multi-pole Debye model to this data. In the process, we obtain the multi-pole Debye coefficients $A_k$ in equation 3.3.

The procedure followed in HFSS to generate broadband material properties from a single set of measurement using Djordjevic-Sarkar model is given here for completeness. First, let us assume that the real part of dielectric constant $\epsilon_1$ and dissipation factor tan $\delta_1$ are available at frequency $f_1$. Then, the frequency dependent real and imaginary parts of relative complex dielectric constant can be generated by following the set of equations below.

\[
K = \frac{\Delta \epsilon}{\ln \left( \frac{\omega_B}{\omega_A} \right)} = \epsilon_1 \tan \delta_1 - \frac{\epsilon_{DC}}{\omega_1 \epsilon_0} \tan^{-1} \left( \frac{\omega_B}{\omega_1} \right) \quad (3.5)
\]

\[
\epsilon_\infty = \epsilon_1 - \frac{K}{2} \ln \left( \left( \frac{\omega_B}{\omega_1} \right)^2 + 1 \right) \quad (3.6)
\]

\[
\Delta \epsilon = 10 \tan \delta_1 \epsilon_\infty \quad (3.7)
\]

\[
\epsilon_{DC} = \Delta \epsilon + \epsilon_\infty \quad (3.8)
\]

\[
\omega_A = \frac{\omega_B}{\epsilon \left( \frac{\omega_B}{\omega_A} \right)} \quad (3.9)
\]

\[
\text{Re} \left[ \epsilon_r(f) \right] = \epsilon_\infty + \frac{K}{2} \ln \left( \frac{\omega_B^2 + \omega^2}{\omega_A^2 + \omega^2} \right) \quad (3.10)
\]

\[
\text{Im} \left[ \epsilon_r(f) \right] = \left( -\frac{1}{\omega_0} \right) \cdot \left( \sigma_{DC} + K \epsilon_0 \omega \left\{ \tan^{-1} \left( \frac{\omega}{\omega_A} \right) - \tan^{-1} \left( \frac{\omega}{\omega_B} \right) \right\} \right) \quad (3.11)
\]

where,

\[\omega\] : angular frequency,

\[\epsilon_\infty\] : real part of relative permittivity at optical frequencies,

\[\epsilon_{DC}\] : real part of relative permittivity at DC,

\[\omega_B = \frac{10^{13}}{2\pi} \text{ Hz}\]

The relaxation frequencies $(1/\tau_k)$ in equation 3.3 are chosen over a large bandwidth (20 kHz
to 200 GHz) and curve fitting is done using non-linear regression. MATLAB’s `nlinfit` function is used in the current study. Figure 3.8 shows a multi-pole Debye model curve fitted to Djordjevic-Sarkar model. The real and imaginary parts of relative permittivity are compared for glass and resin materials between the two models. Eight poles at relaxation frequencies ($1/\tau_k$) equally spaced from 20 KHz to 200 GHz (one each in the decades from 10 kHz to 1 THz) are used for curve-fitting.

Figure 3.8: Multi-pole Debye model curve fitted to Djordjevic-Sarkar Model for Glass and Resin materials.
3.2.2 Implementation of Multi-Pole Debye Model in FDTD

Once the multi-pole Debye coefficients for glass and resin are obtained, we use ADE method in [10] to include material dispersion in FDTD. The polarization current (or the displacement current) in dielectric medium modeled by $P$-pole Debye model, in equation 3.3 is given by equation 3.12:

$$J_{pol} = \sum_{k=1}^{P} \bar{J}_k = j\omega\epsilon_0 \sum_{k=1}^{P} A_k (\epsilon_s - \epsilon_\infty) \frac{\bar{E}}{1 + j\omega \tau_k}.$$  \hspace{1cm} (3.12)

The frequency domain polarization current because of $k^{th}$ pole is given by equation 3.13:

$$\bar{J}_k = j\omega \epsilon_0 A_k (\epsilon_s - \epsilon_\infty) \frac{\bar{E}}{1 + j\omega \tau_k} = j\omega \frac{\zeta_k}{1 + j\omega \tau_k} \bar{E}.$$  \hspace{1cm} (3.13)

Consequently, the Maxwell’s curl equation for magnetic field is modified as in equation 3.14, and the curl equation for electric field remains unmodified as in equation 3.15. Finally, the polarization current of $k^{th}$ pole in equation 3.13 can be transformed to time domain Auxiliary Differential Equation form as in equation 3.16.

$$\nabla \times \bar{H} = \epsilon_0 \epsilon_\infty \frac{\partial}{\partial t} \bar{E} + \sigma_{DC} \bar{E} + \sum_{k=1}^{P} \bar{J}_k.$$  \hspace{1cm} (3.14)

$$\nabla \times \bar{E} = -\mu_0 \mu_r \frac{\partial}{\partial t} \bar{H}.$$  \hspace{1cm} (3.15)

$$\bar{J}_k + \tau_k \frac{\partial \bar{J}_k}{\partial t} = \zeta_k \frac{\partial}{\partial t} \bar{E}.$$  \hspace{1cm} (3.16)

The equations 3.14-3.15 in combination with auxiliary equation 3.16 form the basis for implementing material dispersion in FDTD using multi-pole Debye model. The first two of these equations are discretized in time and space as in conventional FDTD, and the third equation only in time, to obtain a set of update equations for $\bar{E}, \bar{H}, \bar{J}$ respectively. As shown in [10], the update sequence in the FDTD time marching loop is summarized as follows. At every step of the iteration:

1. update magnetic fields using previous magnetic fields (from a full time step ago) and electric fields from previous iteration (from half a time step ago)

2. store the electric fields from previous iteration. These are needed to update polarization currents.
(3) update electric fields using previous electric fields (from a full time step ago), current magnetic fields (from half a time step ago), and sum of previous polarization currents (from a full time step ago).

(4) update polarization currents for each pole using previous polarization currents (from a full time step ago), current electric fields (at the same time step), and stored previous electric fields (from a full time step ago).

The pseudo code of the above steps is shown in equations 3.18-3.19, where $n$ represents the $n^{th}$ time step. The update coefficients are shown in simplified notation for illustration.

\begin{align*}
H^{n+0.5} &= k_1 \cdot H^{n-0.5} + g \cdot E^n \\
temp &= E^n \\
E^{n+1} &= k_2 \cdot E^n + r \cdot H^{n+0.5} + \rho \cdot J^n_k \\
J^{n+1}_k &= k_3 \cdot J^n_k + \sigma \cdot (E^{n+1} - E^n),
\end{align*}

where $g$, $r$, $\sigma$, $\rho$ and $k_{1,2,3}$ are appropriate FDTD update coefficients. As shown above, unlike conventional FDTD, this implementation requires that the electric fields, at least at the cells where there is dispersive material if not all, be stored in computer memory before they are updated. The sequence for updating electric, magnetic fields and polarization currents is shown in the 3.9.

As mentioned earlier, the multi-pole Debye model obtained by curve fitting it to Djordjevic-Sarkar model as shown in section 3.2.1 is implemented using the discretized form of equations 3.14-3.16. In [10], the discretized update equations given for the above equations are for a multi-pole Debye model. These update equations are adapted in this work. This involves calculating polarization currents in equation 3.16 for all the multiple poles we have, one by one and summing them to be used in electric field update equation (discretized form of equation 3.14).
Figure 3.9: Process flow showing sequence of steps involved in implementing dispersive FDTD.

3.3 Glass Weave Skew Analysis using FDTD

The above procedure to include material dispersion in FDTD is applied to analyze the skew induced in PCBs because of glass weave. The glass weave model is implemented as described in section 3.1.2. A PCB model of dimensions 150x100x4.72 mils (milli inches) with a differential pair of microstrip traces is simulated. The traces are 150 mils long, 5.31 mils wide and 2.065 mils thick and are separated edge to edge by 23.89 mils between them. The traces are placed so that one of them falls on the glass fiber bundle and the other fall in between the bundles. The simulation parameters are given in the following table 3.3.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>No of Cells per Wavelength</td>
<td>1020 at 40 GHz (free-space)</td>
</tr>
<tr>
<td>Total Cells including air gaps and CPML</td>
<td>12 million</td>
</tr>
<tr>
<td>Spatial Step: $\Delta x$</td>
<td>7.5 $\mu$m</td>
</tr>
<tr>
<td>Time Step: $\Delta t$</td>
<td>12.9 fsec</td>
</tr>
<tr>
<td>Time Steps</td>
<td>7700</td>
</tr>
<tr>
<td>Grid Truncation</td>
<td>CPML (8 layers)</td>
</tr>
<tr>
<td>Input Pulse</td>
<td>Gaussian Pulse (10% bandwidth of 40 GHz)</td>
</tr>
</tbody>
</table>
Figure 3.10 shows the output pulses on the two traces after traveling 150 mils from FDTD that include material dispersion from glass and resin. As expected, the signal on trace that falls on glass travels slower than that of the trace that falls on resin. The timing skew for this configuration is about 1 psec for 150 mils.

3.4 Comparison with HFSS Simulations

A HFSS model is also built and solved with the finite element solver to benchmark the skew numbers from FDTD. Figure 3.11 shows the models built for FDTD and HFSS.

As mentioned earlier, the broadband frequency domain (0 to 40 GHz) S-parameters (insertion loss for the two traces) are obtained from HFSS and converted to time domain following the procedure shown in figure 3.12. The inverse Fourier transform process mentioned in [49] is used here. Glass weave-induced skew studies using HFSS simulation process can be found in [50,51].

Figure 3.13 shows the time domain pulses obtained from inverse Fourier transform process. The timing skew between the two pulses is 0.97 psec which is a close match to 1 psec obtained from FDTD.
Figure 3.11: Top view of PCB Models for HFSS (left) and FDTD (right).

Figure 3.12: Conversion of S-parameter data to time domain.

The discrete sweep in HFSS from 0 to 40 GHz with a 20 MHz frequency step took around
57.5 hours on a single core (limited by licenses available) of Intel i7-6700 HQ processor running at 2.6 GHz. It consumed about 4.6 GB of RAM. While the FDTD simulation in MATLAB took around 7.97 hours consuming 2.5 GB on the same machine.

3.4.1 Acceleration of FDTD in MATLAB

MATLAB Parallel Computing Toolbox can be leveraged easily to exploit the CUDA-enabled graphical processing unit (GPU) available on a machine. Reasonable speedup over running on a CPU is possible with minimal code changes. The `gpuArrays` are used for storing FDTD fields and update-coefficients. This facilitates running the FDTD update equation on GPU. Vectorized element-wise operations in CPML and Debye update equations can be implemented with `arrayfun()` and `bsxfun()`, which can speed-up the operations further \cite{52}. Significant speedups are possible with CUDA or OpenCL programming which might require specialized knowledge.

The same simulation problem in the above section run on GPU from MATLAB using single precision took around 1.49 hours, a 5x speed-up when compared to CPU implementation, and consumed 1.25 GB of GPU RAM. The GPU on the machine is a NVIDIA GeForce GTX 960M running at 1176 MHz with 640 CUDA Core and graphical RAM of 4 GB running at 5010 MHz. The skew is 1 psec, same as before. Up to 30x speedup are reported for scattering problems with plane wave and dipole antenna excitation in MATLAB \cite{52}. 
Chapter 4

Spherical FDTD Dispersion Relation and Stability Analysis

Spherical FDTD is interesting in the context of modeling conical and spherical structures, and earth-ionosphere system [53], when compared to Cartesian FDTD. The numerical dispersion relationship of an FDTD algorithm predicts the effect of spatial and temporal discretizations on the numerical wave number. It is useful in predicting phase errors in FDTD wave solutions and can be used to choose the optimal grid parameters for a required phase-error tolerance. The numerical dispersion relation for Cartesian FDTD is obtained by substituting plane waves harmonics (elementary functions native to Cartesian coordinates) into the discretized Maxwell’s equations. On the other hand, for Cylindrical FDTD, it is obtained by substituting cylindrical wave harmonics into the discretized Maxwell’s equations [54]. In this chapter, numerical dispersion relation for spherical finite-difference time-domain method (FDTD) based on spherical wave functions (elementary functions native to spherical coordinates) is derived and the sensitivity of numerical wave number with respect to spherical grid parameters is studied. Some sections in the chapter are adapted from our work in [55, 56]. Also, based on the numerical dispersion derived, an attempt is made to derive the stability criterion for spherical FDTD.

4.1 Introduction to Spherical FDTD

Before delving into details of numerical dispersion relation and its derivation, let’s see how the spherical FDTD grid and the corresponding update equations look. Figure 4.1 shows a standard six-faced spherical FDTD unit cell and the locations of electric and magnetic field components
$E_{r,\theta,\phi}$ and $H_{r,\theta,\phi}$ in the grid. The spherical grid is similar to Cartesian FDTD grid shown in figure 1.1 in that the electric fields are along the edges and magnetic fields are normal to the face centers of the unit cell. One major difference though is the curvature of spherical unit cell edges in $\theta$ and $\phi$ directions. As a consequence of this, the size of the unit cell is not constant across the grid, it rather depends on how far the cell is away from the origin.

![Spherical FDTD unit cell showing electric and magnetic field components’ locations.](image)

Figure 4.1: Spherical FDTD unit cell showing electric and magnetic field components’ locations.

### 4.1.1 Spherical FDTD Update Equations

In this section, the update equations for spherical FDTD are revisited. The spherical FDTD update equations are available in different forms in the literature [53], [57], [58], and the ones listed below are adapted mainly from [53]. The discretized update equations in [53], [58] are derived based on Maxwell’s equations in integral form rather than the differential form and are slightly more accurate than the ones in [57].

Let $i,j,k$ represent the indexes in $r,\theta,\phi$ directions respectively. Figure 4.2 shows a unit cell cornered at $(i,j,k)$ and positional offsets of the field components with respect to $(i,j,k)$, similar to Cartesian FDTD. The free-space update equations for $E_{r,\theta,\phi}$ and $H_{r,\theta,\phi}$ can be derived from
source-free modified Ampere’s law and Faraday’s law in integral form, respectively. Considering the latter given in equation 4.2, we observe there are surface and closed-contour integrals.

\[
\varepsilon_0 \frac{d}{dt} \int_S \mathbf{E} \cdot d\mathbf{S} = \oint_C \mathbf{H} \cdot d\mathbf{l} \quad (4.1)
\]

\[
-\mu_0 \frac{d}{dt} \int_S \mathbf{H} \cdot d\mathbf{S} = \oint_C \mathbf{E} \cdot d\mathbf{l} \quad (4.2)
\]

Referring to unit cell in figure 4.2 at \((i, j, k)\), the Faraday’s law for \(H_r\) involves surface integration over bottom surface (to which \(H_r\) is perpendicular to), and closed-contour integral on the edges enclosing that (bottom) surface. The surface integral for \(H_r\), centered at \((i, j + 1/2, k + 1/2)\), can be written as in equation 4.3 and simplified as in equation 4.7 following the procedure below.

\[
\int_S H_r dS = \int_{k\Delta\phi}^{k\Delta\phi + \Delta\phi} \int_{j\Delta\theta - \Delta\theta}^{j\Delta\theta + \Delta\theta} H_r (r d\theta)(r \sin \theta d\phi) \quad (4.3)
\]

\[
= \int_{k\Delta\phi - \Delta\phi}^{k\Delta\phi + \Delta\phi} \int_{j\Delta\theta - \Delta\theta}^{j\Delta\theta + \Delta\theta} H_r r^2 \sin \theta d\theta d\phi \quad (4.4)
\]

\[
= r^2 \Delta\phi H_r \Big|_{(i,j+1/2,k+1/2)} \left[ \cos(j\Delta\theta) - \cos((j + 1)\Delta\theta) \right] \quad (4.5)
\]
\[ 2r^2 \Delta \phi H_r|_{(i,j+\frac{1}{2},k+\frac{1}{2})} \sin \left( j \Delta \theta + \frac{\Delta \theta}{2} \right) \sin \left( \frac{\Delta \theta}{2} \right) \]  
\[ = A_r|_{(i, j+\frac{1}{2})} H_r|_{(i, j+\frac{1}{2}, k+\frac{1}{2})}, \]  
(4.6)  
(4.7)

where \( A_r|_{(i, j+\frac{1}{2})} = 2r^2 \Delta \phi \sin \left((j + \frac{1}{2}) \Delta \theta \right) \sin \left( \frac{\Delta \theta}{2} \right) \) represents the surface area which is a function of radius and elevation angle only (indexes \( i \) and \( j \) only).

And the corresponding contour integral on the right hand side of equation 4.2 (for \( H_r \) term on the left-hand side) is as shown in equation in equation 4.8:

\[
\oint_C \mathbf{E} \cdot d\mathbf{l} = E_\theta|_{(i, j+\frac{1}{2}, k)} \theta|_{(i)} - E_\theta|_{(i, j+\frac{1}{2}, k+1)} \theta|_{(i)} + E_\phi|_{(i, j+1, k+\frac{1}{2})} \phi|_{(i, j+1)} - E_\phi|_{(i, j, k+\frac{1}{2})} \phi|_{(i, j)},
\]
(4.8)

where edge length \( l_\theta|_{(i)} = r \Delta \theta \) is a function of radius (index \( i \) only) and edge length \( l_\phi|_{(i, j)} = r \sin(j \Delta \theta) \Delta \phi \) is a function of radius and elevation angle (indexes \( i \) and \( j \) only). It is noted here that \( r = i \Delta r \).

Similary, the integrals are simplified for other electric and magnetic field components and the spherical FDTD update equations in final form as given in [50] are as follows:

\[
E_r|_{(i+\frac{1}{2}, j, k)}^{n+1} = E_r|_{(i+\frac{1}{2}, j, k)}^{n} + \frac{\Delta t}{\varepsilon_r|_{(i+\frac{1}{2}, j, k)} A_r|_{(i+\frac{1}{2}, j)}} \times
\left[
\left(H_\theta|_{(i+\frac{1}{2}, j, k-\frac{1}{2})}^{n+\frac{1}{2}} - H_\theta|_{(i+\frac{1}{2}, j, k+\frac{1}{2})}^{n+\frac{1}{2}} \right) l_\theta|_{(i+\frac{1}{2})} +
\left(H_\phi|_{(i+\frac{1}{2}, j, k, \frac{1}{2})}^{n+\frac{1}{2}} - H_\phi|_{(i+\frac{1}{2}, j, \frac{1}{2})}^{n+\frac{1}{2}} \right) l_\phi|_{(i+\frac{1}{2}, j, \frac{1}{2})}
\right]
\]
(4.9)

\[
E_\theta|_{(i, j+\frac{1}{2}, k)}^{n+1} = E_\theta|_{(i, j+\frac{1}{2}, k)}^{n} + \frac{\Delta t}{\varepsilon_\theta|_{(i+\frac{1}{2}, j, k)} A_\theta|_{(i+\frac{1}{2}, j)}} \times
\left[
\left(H_r|_{(i+\frac{1}{2}, j, k, \frac{1}{2})}^{n+\frac{1}{2}} - H_r|_{(i+\frac{1}{2}, j, k-\frac{1}{2})}^{n+\frac{1}{2}} \right) l_r -
\left(H_\phi|_{(i+\frac{1}{2}, j, k, \frac{1}{2})}^{n+\frac{1}{2}} - H_\phi|_{(i+\frac{1}{2}, j, \frac{1}{2})}^{n+\frac{1}{2}} \right) l_\phi|_{(i+\frac{1}{2}, j, \frac{1}{2})} +
\left(H_\phi|_{(j+\frac{1}{2}, i+\frac{1}{2}, k)}^{n+\frac{1}{2}} - H_\phi|_{(j+\frac{1}{2}, i, k)}^{n+\frac{1}{2}} \right) l_\phi|_{(j+\frac{1}{2}, i, k)}
\right]
\]
(4.10)

\[
E_\phi|_{(i, j, k+\frac{1}{2})}^{n+1} = E_\phi|_{(i, j, k+\frac{1}{2})}^{n} + \frac{\Delta t}{\varepsilon_\phi|_{(i+\frac{1}{2}, j, k+\frac{1}{2})} A_\phi|_{(i+\frac{1}{2}, j, k+\frac{1}{2})}} \times
\left[
\left(H_r|_{(i, j, \frac{1}{2}, k+\frac{1}{2})}^{n+\frac{1}{2}} - H_r|_{(i, j-\frac{1}{2}, k+\frac{1}{2})}^{n+\frac{1}{2}} \right) l_r +
\left(H_\theta|_{(i, j, \frac{1}{2}, k+\frac{1}{2})}^{n+\frac{1}{2}} - H_\theta|_{(i, j+\frac{1}{2}, k+\frac{1}{2})}^{n+\frac{1}{2}} \right) l_\theta +
\left(H_\phi|_{(j, i+\frac{1}{2}, \frac{1}{2})}^{n+\frac{1}{2}} - H_\phi|_{(j, i, \frac{1}{2})}^{n+\frac{1}{2}} \right) l_\phi
\right]
\]
The expressions for the edge lengths and face areas that appear in the above equations, and shown on the spherical FDTD grid in figure 4.1.1, are given by:

\[
H_{\theta}|_{(i+\frac{1}{2},j,k+\frac{1}{2})} = H_{\theta}|_{(i-\frac{1}{2},j,k+\frac{1}{2})} \Delta \theta \quad (4.11)
\]

\[
H_{r}|_{(i,j+\frac{1}{2},k+\frac{1}{2})} = H_{r}|_{(i,j+\frac{1}{2},k+\frac{1}{2})} \frac{\Delta t/\mu r}{A_{\theta}|_{(i,j+\frac{1}{2})}} \times \left[ (E_{\theta}|_{(i,j+\frac{1}{2},k)} - E_{\theta}|_{(i,j+\frac{1}{2},k+1)}) l_{\theta}|_{(i)} + E_{\phi}|_{(i,j+1,k+\frac{1}{2})} l_{\phi}|_{(i,j)} \right] \quad (4.12)
\]

\[
H_{\phi}|_{(i+\frac{1}{2},j,k+\frac{1}{2})} = H_{\phi}|_{(i+\frac{1}{2},j,k+\frac{1}{2})} \frac{\Delta t/\mu \phi}{A_{\phi|_{(i+\frac{1}{2})}}} \times \left[ (E_{\theta}|_{(i+\frac{1}{2},j,k)} - E_{\theta}|_{(i+\frac{1}{2},j,k+1)}) l_{\theta} - E_{\phi}|_{(i+1,j,k+\frac{1}{2})} l_{\phi}|_{(i,j)} \right] \quad (4.13)
\]

\[
H_{\phi}|_{(i,j+\frac{1}{2},k)} = H_{\phi}|_{(i+\frac{1}{2},j+\frac{1}{2},k)} \frac{\Delta t/\mu \phi}{A_{\phi|_{(i+\frac{1}{2})}}} \times \left[ (E_{\theta}|_{(i,j+\frac{1}{2},k)} - E_{\theta}|_{(i+\frac{1}{2},j+1,k)}) l_{\theta} + E_{\phi}|_{(i+1,j+\frac{1}{2},k)} l_{\phi}|_{(i+1)} - E_{\theta}|_{(i,j+\frac{1}{2},k)} l_{\theta}|_{(i)} \right] \quad (4.14)
\]

The expressions for the edge lengths and face areas that appear in the above equations, and shown on the spherical FDTD grid in figure 4.1.1, are given by:

\[
l_{r} = \Delta r 
\]

\[
l_{\theta}|_{i} = (i \cdot \Delta r) \Delta \theta 
\]

\[
l_{\phi}|_{i,j} = (i \cdot \Delta r) \Delta \phi \sin(j \cdot \Delta \theta) 
\]

\[
A_{r}|_{i,j} = 2(i \cdot \Delta r)^{2} \Delta \phi \sin(\Delta \theta/2) \sin(j \cdot \Delta \theta) 
\]

\[
A_{\theta}|_{i,j} = (i \cdot \Delta r) \Delta r \Delta \phi \sin(j \cdot \Delta \theta) 
\]

\[
A_{\phi}|_{i} = (i \cdot \Delta r) \Delta r \Delta \theta. 
\]

It should be noted that in the above equations for edge lengths and face areas, we can have half integer \(i, j, k\) depending on field component’s location in the grid.
Figure 4.3: Edge lengths and face areas in spherical FDTD grid

Figure 4.4 shows how the spherical coordinate is discretized in radial ($r$), elevation ($\theta$), and azimuthal ($\phi$) directions and just one "\phi-section" is shown for illustration. It also shows how cell sizes vary, i.e., decrease as we move towards, and increase as we move away from the origin. This position-dependence of spherical FDTD cells needs to be carefully accounted for in the numerical dispersion relation and stability criterion derivations.

Figure 4.4: A section of spherical FDTD grid showing discretization in $r$, $\theta$, and $\phi$ directions.
Moreover, because the spherical grid cells converge at singularities (the origin $r = 0$ and poles $\theta = 0, 180^0$), as shown in figure 4.4, there are some special cells in the spherical FDTD whose shape varies from that of the standard cell shown in figure 4.1. These special cells are shown in figure 4.5. It shows four-faced cell at $r = 0, \theta = 0$, five-faced cells at $\theta = 0$ and a five-faced cell possible at $r = 0$. Similarly, four or five-faced cells are also possible at $\theta = 180^0$.

![Special Cells](image)

Figure 4.5: Special cells in spherical FDTD at poles and origin, also shown is a standard six-faced spherical FDTD unit cell.

### 4.2 Numerical Dispersion Relation

This section introduces what numerical dispersion relation is and how it looks for Cartesian FDTD. This section is adapted from our work in [55]. Wave propagation within finite-difference time-domain (FDTD) meshes deviate from continuous space predictions due to the discrete nature of the underlying update equations. For any given FDTD variant, a numerical dispersion relation can be derived by populating its update equations with the corresponding set of elementary wave functions. The resulting relation, which approaches the continuous space at the limit ($\omega^2 \mu \epsilon = \beta^2$ in a lossless medium) faithfully predicts numerical wavenumber solutions. Armed with such knowledge, an optimal selection of mesh and update equations parameters can be ascertained, while controlling the simulation errors. For the standard Cartesian FDTD, the numerical dispersion
relation is obtained by substituting plane wave solutions in the discretized Maxwell's equations to produce:

$$\mu \epsilon D_t^2 = D_x^2 + D_y^2 + D_z^2,$$  \hspace{1cm} (4.21)

where $D_t = j \frac{\sin \omega \Delta t}{\Delta t / 2}$, $D_\zeta = j \frac{\sin \tilde{\beta} \Delta \zeta}{\Delta \zeta / 2}$, $\zeta \rightarrow x, y, z$, where $\Delta x$, $\Delta y$, $\Delta z$ and $\Delta t$ are spatial and temporal discretization steps respectively, and $\tilde{\beta}$ is the numerical wave number. This relation can be solved for $\tilde{\beta}$ for any given set of frequency and discrete step values.

4.3 Derivation of Spherical FDTD Numerical Dispersion Relation

As mentioned earlier, numerical dispersion relation derivation process generally consists of following steps and these are pictorially shown in figure 4.3.

- Express field components in terms of elementary functions native to the coordinate system,
- Substitute the field components in discretized Maxwells curl equations,
- Reduce the set of equations from the above step to obtain numerical dispersion relation.

The figure also shows steps involved for the Cartesian FDTD numerical dispersion relation derivation, as an example, in which a plane wave represented by $e^{(j \omega t - \beta r)}$ is substituted in discretized Maxwell’s equations, and reduced to finally obtain the dispersion relation.

The dispersion relation in spherical FDTD for $TM_r$, transverse magnetic to radial direction, is derived here. The analysis with $TE_r$ mode also results in the same dispersion relation as shown in [50]. The elementary functions for spherical coordinates are the solutions to the Helmholtz equation [60] given in equation 4.22. These elementary functions are given in the equation 4.23 and it consists of spherical Hankel functions (used by Schelkunoff) $\beta rh_{n}^{(2)}(\beta r)$, associated Legendre functions $P_n^m(cos\theta)$ and exponential functions $e^{(-jm\phi)}$ to represent $r$, $\theta$, and $\phi$ dependency, respectively. The function $\beta rh_{n}^{(2)}(\beta r)$ represent an outward traveling wave analogous to $e^{(-j\beta z)}$ traveling along the positive z direction.

$$\frac{\partial^2 A}{\partial r^2} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial A}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 A}{\partial \phi^2} + k^2 A = 0$$  \hspace{1cm} (4.22)
Figure 4.6: Numerical dispersion relation derivation process in general and steps involved in the derivation for Cartesian FDTD

\[ A = \beta rh_n^{(2)}(\beta r)P_n^m(\cos \theta)e^{-j(m\phi - \omega t)} \] (4.23)

The spherical field components’ equations are given in terms of these elementary functions as in equations \[4.24\]-[4.29], [60], [61].

\[
E_r = \frac{1}{j\omega \epsilon} \left( \frac{\partial^2}{\partial r^2} + \beta^2 \right) A = \frac{n(n+1)}{\beta r} P_n^m(\cos \theta)e^{-j(m\phi - \omega t)} \] (4.24)

\[
E_\theta = \frac{1}{j\omega r \sin \theta} \frac{\partial^2 A}{\partial r \partial \theta} = \mathcal{E}_\theta \sin \theta \left( \frac{h_n^{(2)}(\beta r)}{\beta r} + h_n^{(2)'}(\beta r) \right) P_n^m(\cos \theta)e^{-j(m\phi - \omega t)} \] (4.25)

\[
E_\phi = \frac{1}{j\omega r \sin \theta} \frac{\partial^2 A}{\partial r \partial \phi} = \mathcal{E}_\phi \frac{1}{\sin \theta} \left( \frac{h_n^{(2)}(\beta r)}{\beta r} + h_n^{(2)'}(\beta r) \right) P_n^m(\cos \theta)e^{-j(m\phi - \omega t)} \] (4.26)

\[ H_r = 0 \] (4.27)

\[
H_\theta = \frac{1}{r \sin \theta} \frac{\partial A}{\partial \phi} = \mathcal{H}_\theta \frac{1}{\sin \theta} h_n^{(2)}(\beta r) P_n^m(\cos \theta)e^{-j(m\phi - \omega t)} \] (4.28)

\[ H_\phi = \frac{1}{r \partial \theta} \frac{\partial A}{\partial \theta} \]
These field equations in terms of elementary functions are then substituted in spherical update
equations 4.9-4.14. An intermediate step after the substitution is shown in equation 4.30 as a
equation.
\[
\begin{align*}
\frac{e^{j\omega \Delta t / 2} - e^{-j\omega \Delta t / 2}}{\Delta t} \sin \theta \tilde{h}^{(2)}_{n}(\tilde{\beta}r)P_{m}^{n}(\cos \theta) &= \\
-\frac{e^{-jm\Delta \phi / 2} - e^{jm\Delta \phi / 2}}{r \sin \theta \Delta \phi} \frac{\mathcal{E}_{r} \beta \theta}{\beta r}P_{m}^{n}(\cos \theta) \\
+ \frac{N(\tilde{\beta}r^{+}) - N(\tilde{\beta}r^{-})}{r \Delta r} \frac{\mathcal{E}_{\phi}}{\sin \theta}P_{m}^{n}(\cos \theta)
\end{align*}
\] (4.30)

The resultant set of five (not six because \(H_{r} = 0\) for \(TM_{r}\) modes) equations can be concisely
represented in the form of a matrix equation as given below:
\[
\begin{bmatrix}
-\epsilon D_{t} & 0 & 0 & -D_{\phi}^{E} & +D_{\theta}^{E} \\
0 & -\epsilon D_{t} & 0 & 0 & -D_{r}^{E} \\
0 & 0 & -\epsilon D_{t} & +D_{r}^{E} & 0 \\
-D_{\phi}^{H} & 0 & +D_{r}^{H} & -\mu D_{t} & 0 \\
+D_{\theta}^{H} & -D_{r}^{H} & 0 & 0 & -\mu D_{t}
\end{bmatrix}
\begin{bmatrix}
\mathcal{E}_{r} \\
\mathcal{E}_{\phi} \\
\mathcal{E}_{\theta} \\
\mathcal{H}_{\theta} \\
\mathcal{H}_{\phi}
\end{bmatrix}
= 0.
\] (4.31)

The expressions for the above terms are given in equations 4.34-4.40. For a non-trivial field
solution to matrix equation 4.31, the determinant should be made zero as shown in equation 4.32
\[
\det
\begin{bmatrix}
-\epsilon D_{t} & 0 & 0 & -D_{\phi}^{E} & +D_{\theta}^{E} \\
0 & -\epsilon D_{t} & 0 & 0 & -D_{r}^{E} \\
0 & 0 & -\epsilon D_{t} & +D_{r}^{E} & 0 \\
-D_{\phi}^{H} & 0 & +D_{r}^{H} & -\mu D_{t} & 0 \\
+D_{\theta}^{H} & -D_{r}^{H} & 0 & 0 & -\mu D_{t}
\end{bmatrix}
= 0
\] (4.32)

Making the determinant zero finally produces the numerical dispersion relatio 4.33 for spher-
ical FDTD, which is the same dispersion relationship as that for \(TE_{r}\) modes in [56].
\[
\mu \epsilon D_{t}^{2} = D_{r}^{E}D_{r}^{H} + D_{\phi}^{E}D_{\phi}^{H} + D_{\theta}^{E}D_{\theta}^{H},
\] (4.33)
where

\begin{align*}
D_t & = \frac{j \sin \omega \Delta t/2}{\Delta t/2} \\
D_r^E & = \frac{\tilde{\beta}(r + \Delta r) h_n^{(2)}[\tilde{\beta}(r + \Delta r)] - \tilde{\beta} r h_n^{(2)}(\tilde{\beta} r)}{\Delta r \left(h_n^{(2)}(\tilde{\beta} r^+) + \tilde{\beta} r^+ h_n^{(2)}(\tilde{\beta} r^+)\right)}, \\
D_r^H & = \frac{N^+ - N^-}{\tilde{\beta} r \Delta r h_n^{(2)}(\tilde{\beta} r)}, \\
D_\theta^E & = \frac{\beta r h_n^{(2)}(\beta r)}{n(n + 1) \sin \Delta \theta/2} \frac{\Delta \theta/2}{r \sin \theta^+ \Delta \theta P_n^m(\cos \theta^+)} \sin^2(\theta + \Delta \theta) P_n^m[\cos(\theta + \Delta \theta)] - \sin^2 \theta P_n^m(\cos \theta), \\
D_\theta^H & = \frac{\beta r h_n^{(2)}(\beta r)}{n(n + 1) \sin \Delta \theta} \frac{P_n^m(\cos \theta^+) - P_n^m(\cos \theta^-)}{r \sin \theta \Delta \theta P_n^m(\cos \theta)}, \\
D_\phi^E & = -j \frac{\sin m \Delta \phi/2}{\Delta \phi/2} \frac{\Delta \theta/2}{\sin \Delta \theta/2 r^2 \sin^2 \theta^+} \frac{1}{\rho}, \\
D_\phi^H & = -j \frac{\sin m \Delta \phi/2}{\Delta \phi/2}. 
\end{align*}

and

\begin{align*}
N^\pm & = h_n^{(2)}(\tilde{\beta} r^\pm) + \tilde{\beta} r^\pm h_n^{(2)}(\tilde{\beta} r^\pm),
\end{align*}

with \( r^\pm = r \pm \Delta r/2, \theta^\pm = \theta \pm \Delta \theta/2. \)

### 4.3.1 Position Dependence of Numerical Dispersion Relation

This numerical dispersion relation is position-dependent, i.e., a function of absolute position along \( r \) and \( \theta \) directions, an anticipated dependence since mesh cell sizes in spherical FDTD vary with radius and elevation angle, \((r, \theta)\) as shown in figure 4.4.

### 4.3.2 Convergence Analysis

The numerical dispersion relation in 4.33 can be tested for convergence in the farfield where \( r \to \infty \), or in the continuum limit where \( \Delta r, \Delta \theta, \Delta \phi \to 0 \). In the continuum limit, it converges to that of free-space dispersion relation \( \omega^2 \mu \varepsilon = \beta^2 \), and in the farfield it converges to that of in equation 4.42 [56]. If we replace \( \Delta r \) with \( \Delta x \) in this equation, it is essentially same as the dispersion
relation for one-dimensional FDTD in [62].

\[
\frac{\sin \omega \Delta t/2}{\Delta t/2} \frac{\sin \tilde{\beta} \Delta r/2}{\Delta r/2} = \quad (4.42)
\]

where, \( \tilde{\beta} \) is the numerical wave number. This makes total sense because, at larger and larger radii, the spherical FDTD grid appears more and more as a one-dimensional FDTD grid.

### 4.4 Numerical Wave Number Sensitivity Analysis

In this section, the sensitivity of numerical wave number to grid parameters is studied. This analysis will help us understand the errors in wave propagation within spherical FDTD and select better simulation parameters with appropriate error control. This section is adapted from our work [55]. Equation 4.33 is solved for the numerical wavenumber \( \tilde{\beta} \) using \texttt{fsolve} function in MATLAB. The chosen time step \( \Delta t \) is stable expression from [53]:

\[
\Delta t \leq \left[ c \sqrt{l_r^{-2} + l_{\theta}^{-2} + l_{\phi}^{-2}} \right]^{-1}. \quad (4.43)
\]

where \( c \) is the speed of light in vacuum and \( l_r, l_{\theta}, l_{\phi} \) are minimum non-zero edge lengths in the grid.

The resulting numerical wave number is typically complex-valued, especially near the origin, which is a departure from the continuous free-space wave number \( \beta_0 \). This behavior is further studied for different radii, mesh resolutions, elevation angles, and mode numbers.

As the cell size decreases when we approach singularities, origin or poles, the wave number is expected to behave eccentric. And as we move away from the origin towards the farfield, the spherical wave propagation approaches that of one dimensional plane wave. Then, we expect the wave number to approach that of one dimensional FDTD mesh which when sufficiently resolved produces free space wave number.

#### 4.4.1 Sensitivity to Mesh Resolution

The numerical dispersion relation (4.33) is solved for different mesh resolutions \( \Delta r = \lambda_0/R \) where \( R = 10, 20, 40 \) free-space cells per wavelength at a frequency of 1 GHz, \( \Delta \theta = \frac{\pi}{20} \), and
\[ \Delta \phi = \frac{2\pi}{40} \]. The time step \( \Delta t \) is chosen as maximum value of (4.43), where \( l_t = \Delta r \), \( l_{\theta} = \Delta r \Delta \theta \) and \( l_\phi = \Delta r \Delta \phi \sin(\Delta \theta) \). The elevation angle \( \theta \) is chosen as \( \Delta \theta \).

The normalized real and imaginary parts of the numerical wave number with respect to normalized distance from the origin are shown in figure 4.7 for different mesh resolutions. As we move away from the origin, the \( \text{Re}(\tilde{\beta}/\beta_0) \) converges to one signifying the numerical wave number is same as the free space wave number. However, as we move towards the origin, \( \text{Re}(\tilde{\beta}/\beta_0) \) increases beyond unity. This signifies that the wave travels slower than speed of light in free space. The \( \text{Im}(\tilde{\beta}/\beta_0) \) quantity is totally a spurious error and causes either solution attenuation or growth near the origin, depending on its sign. As we approach origin, the wave is initially attenuated and then amplified in close proximity to the origin. Also, as one would expect, figure 4.7 shows that the higher mesh resolutions simulate wave propagation better near the origin.

![Figure 4.7: Real and imaginary parts of wave number vs. normalized distance from origin at different resolutions (\( \theta = \Delta \theta \), \( n = 3 \), and \( m = 0 \)).](image)
4.4.2 Sensitivity to Mode Numbers

Next, the mode numbers \( n \) or \( m \) are varied while keeping the other integer constant. Solutions for higher \( n \) modes get affected more as we move towards the origin for a fixed \( m \) as shown in figure 4.8. The increased sensitivity with increasing \( n \) can be attributed to the fact that higher order Legendre functions vary rapidly with \( \theta \), and become sparsely sampled for a fixed \( \theta \) resolution. For example, when \( m = 0 \), \( P_n^m(\cos \theta) \) for \( n = 1, 2, 3 \) are listed in the table 4.1.

Table 4.1: Legendre Polynomials \( P_n^m(\cos \theta) \) for some lower order \( n \) and \( m = 0 \)

<table>
<thead>
<tr>
<th>( n )</th>
<th>( P_0^0(\cos \theta) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( \cos \theta )</td>
</tr>
<tr>
<td>2</td>
<td>( \frac{1}{2}(3\cos^2 \theta - 1) )</td>
</tr>
<tr>
<td>3</td>
<td>( \frac{1}{2}\cos \theta(5\cos^2 \theta - 3) )</td>
</tr>
</tbody>
</table>

As shown in figure 4.9, it is also observed that the effect of changing \( m \) for a fixed \( n \) is minimal on the behavior of numerical wave number.
Figure 4.9: Real and imaginary parts of wave number vs. normalized distance from origin for different mode numbers $m$. Here $\theta = \Delta \theta$, $R = 40$, and $n = 4$.

### 4.4.3 Sensitivity to Elevation Angle

Figure 4.10 shows wave number sensitivity to different elevation angles, which is relatively minimal compared to radial distance. This is surprising result, as we expect the numerical wave number to show some dependence, if not strong, on $\theta$ because the cell sizes reduce considerably moving towards the poles. This might be because, the edge length $l_{\theta} = r \Delta \theta$ of a cell doesn’t depend on elevation angle ($\theta$) and the FDTD is constrained by this edge length.

### 4.5 Stability Analysis

Having derived the position-dependent numerical dispersion relation and seen its sensitivity in the previous sections, we will attempt to study the stability of spherical FDTD scheme. The stability criterion sets the maximum time step $\Delta t_{\text{max}}$ that we can use in spherical FDTD beyond which the fields will grow unbounded (instability). The stability study is interesting because of the non-uniform grid in spherical FDTD; grid cells are small close to the origin and poles, and grow
larger as we move away from them. Given that, we expect that grid cells close to the origin and poles set the stability condition or criterion for spherical FDTD.

As shown for Cartesian FDTD case in [12], the stability criterion is a by product of numerical dispersion relation. The derivation of stability criterion involve the following steps [63]:

- Obtain numerical dispersion relation
- Obtain temporal and spatial mode growth,
- Apply the condition that maximum spatial mode growth \( \leq \) maximum temporal mode growth. This results in stability criterion (a bound on \( \Delta t \))

Following the above steps for Cartesian FDTD produce:

- Dispersion relation :
  \[
  \left( \sqrt{\varepsilon\mu}\frac{\sin \omega \Delta t/2}{\Delta t/2} \right)^2 = \left( \frac{\sin \beta_x \Delta x/2}{\Delta x/2} \right)^2 + \left( \frac{\sin \beta_y \Delta y/2}{\Delta y/2} \right)^2 + \left( \frac{\sin \beta_z \Delta z/2}{\Delta z/2} \right)^2
  \]

- Maximum temporal mode growth \( \sqrt{\varepsilon\mu} \frac{2}{\Delta t} \)
• Maximum spatial mode growth \( \sqrt{\left(\frac{2}{\Delta x}\right)^2 + \left(\frac{2}{\Delta y}\right)^2 + \left(\frac{2}{\Delta z}\right)^2} \)

• Stability criterion:

\[
\Delta t \leq \frac{\sqrt{c_t}}{\sqrt{\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2 + \left(\frac{1}{\Delta z}\right)^2}} = \Delta t_{\text{max}}. \tag{4.44}
\]

4.5.1 Existing Stability Analysis for Spherical FDTD

Before attempting to obtain stability criterion for spherical FDTD based on the above procedure, existing stability conditions available in the literature are reviewed.

1. One such condition is available in [53]. The stability condition is given as below:

\[
\Delta t \leq \frac{1}{c \cdot \sqrt{l_r^{-2} + l_{\theta}^{-2} + l_{\phi}^{-2}}} \tag{4.45}
\]

where, \( l_r = \Delta r, \ l_{\theta} = r_{\text{min}} \Delta \theta, \ l_{\phi} = r_{\text{min}} \sin \Delta \theta \Delta \phi \) are the minimum edge lengths of Yee cells in the problem space.

This is an approximate stability criterion directly adapted from Cartesian FDTD grid’s given in equation [4.44]. And there is no dispersion relation associated with it.

2. The next one is given in [64]. The numerical dispersion relation leading to this stability criterion is obtained by substituting plane wave solutions in spherical FDTD update equations and the criterion is given below:

\[
c \Delta t \leq \frac{c_1 \Delta l}{N \sin^2 \left(\frac{\pi}{4N}\right)} \tag{4.46}
\]

where,

• \( c_1 \) is a constant (no expression given),

• \( \Delta l = \frac{\pi R}{N} \sin \left(\frac{\pi}{2N}\right) = \frac{R\sin(\Delta \theta) \Delta \phi}{2} \) the “smallest distance between cells”,

• \( R \) is the radius of Earth,

• the stability condition is valid only when \( \Delta r \gg \Delta l \),

• when \( \Delta r \ll \Delta l \), “the stability limit is determined mainly by \( \Delta r \)”
• $2N$, $N$ are the number of points in longitude and latitude directions.

3. The third one is available in [65].

$$\Delta t \leq \frac{1}{c} \sqrt{\frac{1}{(\Delta r)^2} + \frac{1}{4(\Delta r \Delta \theta)^2} + \frac{1}{4(\Delta r \Delta \phi \sin \Delta \theta)^2}} \quad (4.47)$$

This stability condition does not depend on absolute radial position ($r$) in the grid. Again, the Numerical Dispersion relation is obtained by substituting plane wave solutions in Spherical FDTD update equations.

### 4.5.2 Stability Criterion based on Position Dependent Numerical Dispersion Relation

Having seen the stability conditions available in the literature, an attempt is made to obtain the stability criterion for spherical FDTD from position dependent numerical dispersion relation derived earlier in the chapter. The dispersion relation given in equation [4.33](#) is repeated here for convenience:

$$\mu \epsilon D_t^2 = D_r^E D_r^H + D_\theta^E D_\theta^H + D_\phi^E D_\phi^H, \quad (4.48)$$

The condition for stability is that the maximum spatial mode growth should be less than or equal to the maximum temporal mode growth, i.e.,

$$|D_r^E D_r^H|_{\text{max}} + |D_\theta^E D_\theta^H|_{\text{max}} + |D_\phi^E D_\phi^H|_{\text{max}} \leq |\mu \epsilon D_t^2|_{\text{max}} \quad (4.49)$$

where $|\mu \epsilon D_t^2|_{\text{max}} = \mu \epsilon \left( \frac{2}{\Delta t_{\text{max}}} \right)^2$. Therefore, the stability criterion can be written as:

$$\Delta t_{\text{max}} = \frac{\Delta r \sqrt{\mu \epsilon}}{\tau} \quad ; \tau = \frac{\Delta r}{2} \sqrt{|D_r^E D_r^H|_{\text{max}} + |D_\theta^E D_\theta^H|_{\text{max}} + |D_\phi^E D_\phi^H|_{\text{max}}} \quad (4.50)$$

For a given mode $(n, m)$, we calculate $\tau$ as given in above expression and obtain theoretical $\Delta t_{\text{max}}$. One can notice from figure [4.4](#) that as we move away from the origin, the cell sizes increase and we expect the stability criterion to loosen. The stability criterion can also be observed practically by setting a simple free space simulation problem, and by using the update equations [4.9]-[4.14](#) we can vary time step size and observe the threshold $\Delta t$ ($\Delta t_{\text{max}}$) below which the fields
are bounded and above which the fields grow unbounded. We can exclude grid cells near origin by making them part of PEC (all the fields are zero inside it and tangential electric fields are zero on the surface). Figure 4.5.2 shows such a problem space which contains PEC sphere at its center. The radius of this sphere is varied and the stability is observed practically.

Figure 4.5.2: Problem space that excludes regions around origin to observe stability criterion practically for spherical FDTD.

Figure 4.5.2 show how stability criterion varies as the PEC size is increased. As expected, the stability criterion becomes less stringent ($\tau$ decreases and so $\Delta t_{\text{max}}$ increases by virtue of equation 4.50). Also, the figure show how stability criterion changes when $\Delta \theta$ changes, i.e., for different discretizations in elevation angle. When the grid is made coarser ($\Delta \theta_2$), we can observe that the stability becomes less stringent compared to finer grid case ($\Delta \theta_1$).

As mentioned earlier, the elementary functions in spherical co-ordinates are composed of Lengendre functions ($P_n^m(\cos \theta)$) and spherical Hankel functions ($h_n^{(1,2)}(\beta r)$). Higher order $n$ and $m$ causes these functions to fluctuate more, and so the need for higher grid resolution for these higher-order functions to get sampled enough. So, we expect the higher-order modes to have stringent stability criterion than the lower-order modes. This is shown in figure 4.5.2 where theoretical $\tau$ is plotted for different central PEC sphere radius at different $n$ and fixed $m = 0$. From the figure, we can see that higher-order modes (higher $n$) have stringent stability criterion (larger $\tau$) than the lower-order modes. Also shown is the observed $\tau$ in addition to the theoretically obtained $\tau$. 
Surprisingly, the observed $\tau$ does not show correspondence to any one particular mode. Even though, the excitation pattern is changed to excite a particular mode $(n, m)$ in the grid, the stability criterion didn’t change, hence a single curve for observed $\tau$. As the smallest cell size increases (i.e., as PEC sphere radius increases), the observed stability factor $\tau$ decreases slower than the modes’ theoretical stability factors. It appeared as if a combination of modes is getting excited in the grid and the mode mixture is controlling the stability.

Figure 4.12: Practically observed stability criterion for different PEC sphere radii and for different $\Delta \theta$.

Figure 4.13: Theoretical stability factor $\tau$ at various PEC sphere radii for different modes $n, m = 0$. Also shown is the observed $\tau$. 
4.5.3 Challenges in Validating Stability Criterion

Exploring the reasons why the observed \( \tau \) didn’t match the theoretical \( \tau \) might lead one to the following questions.

- How to excite a single mode \((n,m)\) to verify the stability criterion?
- How to find the highest-order mode being excited that might be deciding the stability criterion?
- Is stability criterion same for all modes with same \( n \)?
- Is it possible that the algorithm renders different mode number \((n)\) for Legendre and Spherical Hankel Functions?
- What is the effect of radial node number \((p)\)?

To address the first question of the above, we need spherical FDTD update equations for a single mode \((n,m)\) as was done for BOR FDTD (2-dimensional cylindrical FDTD) in [54]. In the literature for spherical FDTD, the mode specific update equations are discussed and derived in [66]. An attempt was made to obtain the stability criterion as well in that work. Nonetheless, the theoretical and observed stability criterion fail to obey and finally an estimate based on heuristic fit (empirical fit) is obtained for a stability factor \( B \) (analogous to \( \tau \) in this work), and it was shown that the observed stability factor lies close to this value. So, the perfect stability criterion for spherical FDTD remains still elusive. Also, it was shown that the observed and estimated stability factors both scale linearly with \( n \) and show little dependence on \( m \).

For obtaining the maximum value under the square root in equation [4.50], the numerical wave number must be used which in turn is obtained from solving the numerical dispersion relation. However, in the work mentioned above, the free space wave number is used instead. One can enhance the stability estimate (of aforementioned work) by obtaining the numerical dispersion on similar lines to this present work and using the numerical wave number to obtain the stability factor.
Chapter 5

Spherical FDTD PML Analysis

This chapter deals with the Perfectly Matched Layer (PML) implementation and its absorption analysis for spherical FDTD. As mentioned in introductory chapter, PML is an effective Absorbing Boundary Condition (ABC) to truncate FDTD grids and was introduced by Berenger in 1994 \cite{5,12}. Berenger introduced the PML in split-field form for Cartesian FDTD, where each of the six field components are split into two orthogonal components \cite{12}. Later, PML has been re-interpreted as anisotropic uniaxial medium (UPML) by Gedney \cite{6} and in stretched-coordinate form independently by Chew-Weedon \cite{30} and Rappaport \cite{31}.

5.1 Perfectly Matched Layer in Spherical FDTD

The PML has been extended to spherical FDTD by Teixeira \cite{67,68} in 1997 using the stretched-coordinate form of PML. However, complete discretized equations for stretched-coordinate PML implementation in spherical FDTD remained unavailable in the literature until recently. Recent work by Bao and Teixeria tried to fill this gap. The authors analyzed the performance of PML in absorbing the incident waves in spherical FDTD \cite{69,70}, while the discretized PML equations are available in \cite{70}. However, these discretized equations contain typographical errors making it hard to make use of them to implement PML in spherical FDTD. Moreover, the above works were based on backward difference in PML region. Here in this work, the discretized PML equations (based on stretched-coordinate formulation for spherical coordinates) are based on central-differencing as in the non-PML region.
In addition to the above, the absorption capabilities of the stretched-coordinate PML are analyzed and compared with split-field PML formulation. Also, a closed-form expression for reflection coefficient is derived for continuous space PML in spherical coordinates that acts as a benchmark for the comparing effectiveness of different formulations. Moreover, the efficacy of a lossy absorbing shell, where a lossy medium is used to absorb waves similar to implementation in [29], to truncate spherical FDTD grid is analyzed. It will be shown clearly why split-field implementation of PML is not as effective in truncating spherical FDTD and is not as efficient absorber as it is in Cartesian FDTD. It is also shown that split-field PML is only as efficient as lossy absorbing shell in spherical FDTD.

5.2 Split-Field PML Formulation

The split-field PML in Cartesian FDTD involves splitting the field component perpendicular to normal of PML surface into orthogonal portions: one that propagates along the normal to the PML surface and one that propagates perpendicular to the normal. The portion that propagates in the direction of normal to the PML surface is applied a loss factor in the form of electrical conductivity $\sigma$ ($\sigma_e$) or magnetic conductivity $\sigma^*$ ($\sigma_m$) and gets absorbed by the PML.

The PML boundary condition in spherical FDTD has the following properties: (a) it surrounds the problem space as shown in figure 5.1 (in the form of a shell around an hazelnut or similar to thick rind surrounding red/pink flesh of a watermelon), and (b) the spherical FDTD PML region is made of layers (because of radial discretization in spherical FDTD) and normals to these layers are parallel to radial direction. Therefore, we have a scenario similar to split-field PML implementation in Cartesian coordinates. Similar to Cartesian case, the field components perpendicular to the normal of the PML surface are split into two orthogonal portions. This means that only the components other than the radial component, i.e $X_{\theta,\phi}$ are split into $X_{\theta r,\theta \phi}$ and $X_{\phi r,\phi \theta}$, in split-field PML implementation for spherical FDTD. Here, $X$ represents both electric and magnetic fields. The portions $X_{\theta r}$ and $X_{\phi r}$ are applied the PML artificial loss factors $\sigma_r$ and $\sigma^*_r$ in spherical FDTD, where they satisfy the condition $\frac{\sigma_r}{\epsilon} = \frac{\sigma^*_r}{\mu}$. 
Figure 5.1: PML boundary condition surrounding problem space in spherical FDTD.

This way of field components’ split is evident from the equation sets 5.1-5.6 and 5.7-5.14. The first set is the Maxwell’s equations in differential form in spherical coordinates.

\[
\begin{align*}
\frac{\epsilon}{r} \frac{\partial E_r}{\partial t} &= \frac{1}{r \sin \theta} \left[ \frac{\partial (\sin \theta H_{\phi})}{\partial \theta} - \frac{\partial H_{\theta}}{\partial \phi} \right] \\
\frac{\epsilon}{r} \frac{\partial E_{\theta}}{\partial t} &= \frac{1}{r} \left[ \frac{1}{\sin \theta} \frac{\partial H_r}{\partial \phi} - \frac{\partial (r H_{\phi})}{\partial r} \right] \\
\frac{\epsilon}{r} \frac{\partial E_{\phi}}{\partial t} &= \frac{1}{r} \left[ \frac{\partial (r H_{\theta})}{\partial r} - \frac{\partial H_r}{\partial \theta} \right] \\
-\mu \frac{\partial H_r}{\partial t} &= \frac{1}{r \sin \theta} \left[ \frac{\partial (\sin \theta E_{\phi})}{\partial \theta} - \frac{\partial E_{\theta}}{\partial \phi} \right] \\
-\mu \frac{\partial H_{\theta}}{\partial t} &= \frac{1}{r} \left[ \frac{1}{\sin \theta} \frac{\partial E_r}{\partial \phi} - \frac{\partial (r E_{\phi})}{\partial r} \right] \\
-\mu \frac{\partial H_{\phi}}{\partial t} &= \frac{1}{r} \left[ \frac{\partial (r E_{\theta})}{\partial r} - \frac{\partial E_r}{\partial \theta} \right]
\end{align*}
\]

The second set below is the split-field formulation for PML in spherical FDTD. The fields \( E_{\theta,\phi} \) and \( H_{\theta,\phi} \) are split and only \( E_{\theta r}, E_{\phi r}, H_{\theta r}, H_{\phi r} \) (the portions that propagate in radial direction) are applied the loss factors \( \sigma_r \) or \( \sigma_r^* \) as shown in equations 5.8, 5.10, 5.12, and 5.14. We can also observe that these equations have \( \frac{\partial}{\partial r} \) on the right hand side, signifying the field component portion on the left hand side of these equations propagates along radial \( (r) \) direction. These split-field equations and their discretized versions are available in the chapter 71.

\[
\begin{align*}
\epsilon \frac{\partial E_{\theta r}}{\partial t} &= \frac{1}{r \sin \theta} \frac{\partial H_r}{\partial \phi} \\
\epsilon \frac{\partial E_{\phi r}}{\partial t} + \sigma_r E_{\phi r} &= -\frac{1}{r} \frac{\partial (r H_{\phi})}{\partial r}
\end{align*}
\]
$$\epsilon \frac{\partial E_{\phi \theta}}{\partial t} = -\frac{1}{r} \frac{\partial H_r}{\partial \theta}$$  \hspace{1cm} (5.9) $$

$$\epsilon \frac{\partial E_{\phi r}}{\partial t} + \sigma_r E_{\phi r} = \frac{1}{r} \frac{\partial (rH_\theta)}{\partial r}$$  \hspace{1cm} (5.10) $$

$$-\mu \frac{\partial H_{\theta \phi}}{\partial t} = \frac{1}{r \sin \theta} \frac{\partial E_r}{\partial \phi}$$  \hspace{1cm} (5.11) $$

$$-\mu \frac{\partial H_{\theta r}}{\partial t} - \sigma^*_r H_{\theta r} = -\frac{1}{r} \frac{\partial (rE_\phi)}{\partial \theta}$$  \hspace{1cm} (5.12) $$

$$-\mu \frac{\partial H_{\phi \theta}}{\partial t} - \sigma^*_r H_{\phi r} = \frac{1}{r} \frac{\partial (rE_\theta)}{\partial r}$$  \hspace{1cm} (5.13) $$

5.3 Lossy Absorbing Shell as a Boundary Condition

Absorbing shell is a poor man’s absorbing boundary condition, where the inner region is surrounded by a lossy medium. This lossy medium absorbs the incident waves, reflecting only a part of the incident wave. In Cartesian coordinates, this technique \[29\] perfectly absorbs the incident waves only for normal incidence \[12\]. Therefore, it is interesting to study its behaviour in spherical coordinates. In this section, the spherical FDTD equations given in \[53\] are modified to include the loss factors $\sigma_e$ and $\sigma^*$ that satisfy the reflection-less condition $\frac{\sigma_e}{\epsilon_0} = \frac{\sigma^*}{\mu_0}$. These modified update equations are listed in equations \[5.15\] to \[5.20\]. The performance of this absorbing shell boundary condition is compared with PML formulations later in the chapter.

$$E_r|_{i+\frac{1}{2},j,k}^{n+1} = \left(1 - \frac{\Delta t \sigma_e}{2 \epsilon_0} \right) E_r|_{i+\frac{1}{2},j,k}^{n} + \frac{\Delta t}{\epsilon_r|_{i+\frac{1}{2},j,k} A_r|_{i+\frac{1}{2},j,k}} \left(1 + \frac{\Delta t \sigma_e}{2 \epsilon_0} \right) \times$$

$$\left[ (H_\theta|_{i+\frac{1}{2},j,k-\frac{1}{2}} - H_\theta|_{i+\frac{1}{2},j,k+\frac{1}{2}}) l_{\phi}|_{i+\frac{1}{2},j} + \frac{1}{2} + H_\phi|_{i+\frac{1}{2},j-\frac{1}{2},k} - H_\phi|_{i+\frac{1}{2},j+\frac{1}{2},k} l_{\phi}|_{i+\frac{1}{2},j-\frac{1}{2}} \right]$$  \hspace{1cm} (5.15) $$

$$E_\theta|_{i,j+\frac{1}{2},k}^{n+1} = \left(1 - \frac{\Delta t \sigma_e}{2 \epsilon_0} \right) E_\theta|_{i,j+\frac{1}{2},k}^{n} + \frac{\Delta t}{\epsilon_\theta|_{i,j+\frac{1}{2},k} A_\theta|_{i,j+\frac{1}{2},k}} \left(1 + \frac{\Delta t \sigma_e}{2 \epsilon_0} \right) \times$$

$$\left[ (H_r|_{i,j+,\frac{1}{2},k-\frac{1}{2}} - H_r|_{i,j+,\frac{1}{2},k+\frac{1}{2}}) l_{\phi}|_{i+\frac{1}{2},j} + \frac{1}{2} - H_\phi|_{i+\frac{1}{2},j-\frac{1}{2},k} l_{\phi}|_{i+\frac{1}{2},j+\frac{1}{2}} \right]$$  \hspace{1cm} (5.16)
\[ \begin{align*}
E_{\phi|_{i,j,k+\frac{1}{2}}}^{n+1} & = \left( 1 - \frac{\Delta t \sigma_\rho}{2 \rho_0} \right) E_{\phi|_{i,j,k+\frac{1}{2}}}^{n+1} + \frac{\Delta t}{r_{i,j,k+\frac{1}{2}}^2} + \varepsilon_{\phi|_{i,j,k+\frac{1}{2}}} A_{\phi|_{i}} \left( 1 + \frac{\Delta t \sigma_\rho}{2 \rho_0} \right) \times \\
& \left[ (H_r|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}} - H_r|_{i,j,k+\frac{1}{2}}^{n+\frac{1}{2}}) + \\
H_{\theta|_{i,j,k+\frac{1}{2}}}^{n+\frac{1}{2}} l_{\theta|_{i}} - H_{\theta|_{i,j,k+\frac{1}{2}}}^{n+\frac{1}{2}} l_{\theta|_{i}} \right] \\
H_r|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} & = \left( 1 - \frac{\Delta t \sigma_\rho^*}{2 \rho_0} \right) H_r|_{i,j+\frac{1}{2},k+\frac{1}{2}}^{n+\frac{1}{2}} - \frac{\Delta t / \mu_r}{r_{i,j+\frac{1}{2},k+\frac{1}{2}}} \times \\
& \left[ (E_r|_{i,j+\frac{1}{2},k+1}^{n+1} - E_r|_{i,j+\frac{1}{2},k+1}^{n+1}) l_{r|_{i}} - \\
E_{\phi|_{i,j,k+\frac{1}{2}}}^{n+1} l_{\phi|_{i,j+1}} + E_{\phi|_{i,j,k+\frac{1}{2}}}^{n+1} l_{\phi|_{i,j+1}} \right] \\
H_{\phi|_{i,j+\frac{1}{2},k+\frac{1}{2}}}^{n+\frac{1}{2}} & = \left( 1 - \frac{\Delta t \sigma_\rho^*}{2 \rho_0} \right) H_{\phi|_{i,j+\frac{1}{2},k+\frac{1}{2}}}^{n+\frac{1}{2}} - \frac{\Delta t / \mu_{\phi}}{r_{i,j+\frac{1}{2},k+\frac{1}{2}}} \times \\
& \left[ (E_r|_{i,j+\frac{1}{2},k+1}^{n+1} - E_r|_{i,j+\frac{1}{2},k+1}^{n+1}) l_{r|_{i}} + \\
E_{\theta|_{i+1,j+\frac{1}{2},k+\frac{1}{2}}}^{n+1} l_{\theta|_{i+1}} - E_{\theta|_{i,j+\frac{1}{2},k+\frac{1}{2}}}^{n+1} l_{\theta|_{i+1}} \right],
\end{align*} \]

where,

\[ \begin{align*}
l_r & = \Delta r \\
l_{\theta|_{i}} & = r_{i} \Delta \theta \\
l_{\phi|_{i,j}} & = r_{i} \Delta \phi \sin \theta_{|_{j}} \\
A_r|_{i,j} & = 2r_{i}^2 \Delta \phi \sin(\Delta \theta / 2) \sin \theta_{|_{j}} \\
A_{\theta|_{i,j}} & = r_{i} \Delta r \Delta \phi \sin \theta_{|_{j}} \\
A_{\phi|_{i}} & = r_{i} \Delta r \Delta \theta.
\end{align*} \]
5.4 Stretched-Coordinate PML Formulation

This section covers the theory behind implementation of stretched-coordinate PML in spherical FDTD. The electric and magnetic field update equations in PML region are derived. The notations for the variables and derivation process of the PML update equation are adapted from [69].

5.4.1 Electric Field Stretched-Coordinate PML Equation

Frequency domain Ampere’s law in complex coordinate space, stretched only along radial direction, in spherical coordinate system are given by (similar to Faraday’s equation in [68]):

\[
\begin{align*}
\jmath \omega \epsilon E_r(\omega) &= \frac{1}{\bar{r} \sin \theta} \left[ \frac{\partial}{\partial \theta} (\sin \theta H_\phi(\omega)) - \frac{\partial}{\partial \phi} H_\theta(\omega) \right] \\
\jmath \omega \epsilon E_\theta(\omega) &= \frac{1}{\bar{r}} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (H_r(\omega)) - \frac{\partial}{\partial \bar{r}} (\bar{r} H_\phi(\omega)) \right] \\
\jmath \omega \epsilon E_\phi(\omega) &= \frac{1}{\bar{r}} \left[ \frac{\partial}{\partial \bar{r}} (\bar{r} H_\theta(\omega)) - \frac{\partial}{\partial \theta} H_r(\omega) \right],
\end{align*}
\]

where,

\[
\bar{r}(r, \omega) = \int_0^r s_r(r', \omega) \, dr',
\]

\[
s_r(r, \omega) = a_r(r) + \frac{\sigma_r(r)}{\jmath \omega \epsilon}.
\]

Here, \(\sigma_r\) is the electrical conductivity in radial direction analogous to \(\sigma_{x,y,z}\) for Cartesian FDTD PML. \(s_r(r, \omega)\) is the stretched-coordinate variable for radial direction, and \(\bar{r}(r, \omega)\) is the complex radius variable. Given these, complex radius variable in equation 5.30 can be rewritten as:

\[
\bar{r}(r, \omega) = \int_0^r \left( a_r(r') + \frac{\sigma_r(r')}{\jmath \omega \epsilon} \right) \, dr' = b_r(r) + \frac{\Delta_r(r)}{\jmath \omega \epsilon},
\]

where \(\Delta_r(r) = \int_0^r \sigma_r(r') \, dr'\), not to be confused with radial discretization \(\Delta r\).

Also, it is observed from equation 5.30 that the relationship between partial derivatives in complex and real space is given by:

\[
\frac{\partial}{\partial \bar{r}} = \frac{\partial}{\partial r} \cdot \frac{\partial r}{\partial \bar{r}} = \frac{1}{s_r} \frac{\partial}{\partial r}.
\]
Applying the above manipulations to the equations (5.27-5.29), and after some rearrangement, we get:

\[ j\omega r(\omega)\epsilon E_r(\omega) = \frac{1}{\sin \theta} \left[ \frac{\partial}{\partial \theta} (\sin \theta H_\phi(\omega)) - \frac{\partial}{\partial \phi} H_\theta(\omega) \right], \tag{5.34} \]

\[ j\omega s_r(\omega)\epsilon \tilde{E}_\theta(\omega) = \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (s_r(\omega) \cdot H_r(\omega)) - \frac{\partial}{\partial r} \tilde{H}_\phi(\omega), \tag{5.35} \]

\[ j\omega s_r(\omega)\epsilon \tilde{E}_\phi(\omega) = \frac{\partial}{\partial r} \tilde{H}_\theta(\omega) - \frac{\partial}{\partial \theta} (s_r(\omega) \cdot H_r(\omega)). \tag{5.36} \]

In the above equations, new field terms in stretched-coordinate PML region have been used and they are defined as:

\[ \tilde{H}_{\theta,\phi}(\omega) = \bar{r}(\omega) H_{\theta,\phi}(\omega), \tag{5.37} \]

\[ \tilde{E}_{\theta,\phi}(\omega) = \bar{r}(\omega) E_{\theta,\phi}(\omega). \tag{5.38} \]

Till now all the equations are given in frequency domain. However, they need to be transformed to time domain for FDTD implementation. In time domain, the above equations translate to:

\[ \epsilon \left( b_r(r) \frac{\partial}{\partial t} + \frac{\Delta_v(r)}{\epsilon} \right) E_r(t) = \frac{1}{\sin \theta} \left[ \frac{\partial}{\partial \theta} (\sin \theta H_\phi(t)) - \frac{\partial}{\partial \phi} (H_\theta(t)) \right], \tag{5.39} \]

\[ \epsilon \left( a_r(r) \frac{\partial}{\partial t} + \frac{\sigma_r(r)}{\epsilon} \right) \tilde{E}_\theta(t) = \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (s_r(t) \cdot H_r(t)) - \frac{\partial}{\partial r} (\tilde{H}_\phi(t)), \tag{5.40} \]

\[ \epsilon \left( a_r(r) \frac{\partial}{\partial t} + \frac{\sigma_r(r)}{\epsilon} \right) \tilde{E}_\phi(t) = \frac{\partial}{\partial r} (\tilde{H}_\theta(t)) - \frac{\partial}{\partial \theta} (s_r(t) \cdot H_r(t)). \tag{5.41} \]

\[ H_{\theta,\phi}(t) = \bar{r}^{-1}(t) * \tilde{H}_{\theta,\phi}(t), \tag{5.42} \]

\[ E_{\theta,\phi}(t) = \bar{r}^{-1}(t) * \tilde{E}_{\theta,\phi}(t). \tag{5.43} \]

The frequency domain terms \(s_r(r, \omega)\) and \(\bar{r}(\omega)\), given by equations 5.31 and 5.32 respectively, too are converted to time domain as follows:

\[ s_r(r, t) = F^{-1} \left( a_r(r) + \frac{\sigma_r(r)}{j\omega \epsilon} \right) = a_r(r) \delta(t) + \frac{\sigma_r(r)}{\epsilon} u(t), \tag{5.44} \]

\[ \bar{r}^{-1}(t) = F^{-1} \left( \frac{1}{b_r(r) + \frac{\Delta_v(r)}{j\omega \epsilon}} \right) = \frac{1}{b_r(r)} F^{-1} \left( \frac{j\omega}{b_r(r) + \frac{\Delta_v(r)}{j\omega \epsilon}} \right), \tag{5.45} \]

\[ = \frac{1}{b_r(r)} \frac{d}{dt} \left( e^{-\frac{\Delta_v(r)}{b_r(r) \epsilon}} u(t) \right). \]
Defining $\frac{b_r(r)}{\Delta r(r)} = \tau_0(r)$, we can write equation 5.45 as follows:

$$\bar{r}^{-1}(t) = \frac{1}{b_r(r)} \left( e^{-\frac{t}{\tau_0(r)}} \delta(t) - \frac{1}{\tau_0(r)} e^{-\frac{t}{\tau_0(r)}} u(t) \right)$$ (5.46)

$$= \frac{1}{b_r(r)} \left( \delta(t) - \frac{1}{\tau_0(r)} e^{-\frac{t}{\tau_0(r)}} u(t) \right).$$ (5.47)

Following this conversion to time domain, the convolution operation in the equations (5.39-5.43) is expanded in time domain integral form as follows:

$$s_r(t) * H_r(t) = a_r(r) H_r(t) + \frac{\sigma_r(r)}{\epsilon} \int_0^t H_r(t - t') dt',$$

$$\bar{r}^{-1}(t) * \bar{E}_\theta(t) = \bar{E}_\theta(t)$$

$$= \frac{1}{b_r(r)} \left( \bar{E}_\theta(t) - \frac{1}{\tau_0(r)} \int_0^t \bar{E}_\theta(t - t') e^{-\frac{t'}{\tau_0(r)}} dt' \right)$$ (5.49)

The integral in the above equation is implemented in discrete time domain for FDTD using piece-wise constant summation as:

$$\frac{1}{\tau_0(r)} \int_0^t \bar{E}_\theta(t - t') e^{-\frac{t'}{\tau_0(r)}} dt' \approx \frac{1}{\tau_0(r)} \sum_{n=0}^{n=m} \left( \int_{n\Delta t}^{(n+1)\Delta t} e^{-\frac{t'}{\tau_0(r)}} dt' \bar{E}_\theta(m\Delta t - n\Delta t) \right)$$

$$= (1 - e^{-\frac{\Delta t}{\tau_0(r)}}) \sum_{n=0}^{n=m} e^{-\frac{n\Delta t}{\tau_0(r)}} \bar{E}_\theta(m\Delta t - n\Delta t)$$ (5.50)

The summation in the above equation can be implemented recursively as follows:

$$(1 - e^{-\frac{\Delta t}{\tau_0(r)}}) \sum_{n=0}^{n=m} e^{-\frac{n\Delta t}{\tau_0(r)}} \bar{E}_\theta(m\Delta t - n\Delta t) = (1 - e^{-\frac{\Delta t}{\tau_0(r)}})Q(n\Delta t),$$ (5.51)

where,

$$Q(n\Delta t) = \bar{E}_\theta(n\Delta t) + e^{-\frac{n\Delta t}{\tau_0(r)}} Q((n - 1)\Delta t), Q(0\Delta t) = 0.$$ (5.52)

This recursive summation is efficient for implementation in FDTD schemes as it involves reusing previous summation in the current time step.

Finally, the update equations for FDTD implementation of the time domain stretched-
coordinate PML equations (5.39-5.43) are given by:

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

\[
C_{erh}(i, j, k) \left[ \frac{H_{\phi}^{n+\frac{1}{2}}(i, j, k) \sin(j^+ \Delta \theta) - H_{\phi}^{n+\frac{1}{2}}(i, j - 1, k) \sin(j^- \Delta \theta)}{\Delta \theta} - \frac{H_{\theta}^{n+\frac{1}{2}}(i, j, k) - H_{\theta}^{n+\frac{1}{2}}(i, j, k - 1)}{\Delta \phi} \right],
\] (5.53)

\[
C_{erh}(i, j, k) = \frac{\Delta t \Delta \theta}{2 \sin(j \Delta \theta) \epsilon(i, j, k) \sin(\frac{\Delta \theta}{2})};
\]

\[
\bar{E}_{\theta}^{n+1}(i, j, k) = \frac{1}{a_{r}(i) + \frac{\Delta t \sigma_{r}(i)}{2\epsilon}} \left\{ \left( a_{r}(i) - \frac{\Delta t \sigma_{r}(i)}{2\epsilon} \right) \bar{E}_{\theta}^{n}(i, j, k) + \right.
\]

\[
C_{eth}(i, j, k) \left[ \frac{1}{\Delta \phi \sin(j^+ \Delta \theta)} \left( a_{r}(i) \left[ H_{r}^{n+\frac{1}{2}}(i, j, k) - H_{r}^{n+\frac{1}{2}}(i, j, k - 1) \right] + \frac{\sigma_{r}(i)}{\epsilon} \left[ H_{rs}^{n+\frac{1}{2}}(i, j, k) - H_{rs}^{n+\frac{1}{2}}(i, j, k - 1) \right] \right) - \frac{\bar{H}_{r}^{n+\frac{1}{2}}(i, j, k) - \bar{H}_{r}^{n+\frac{1}{2}}(i - 1, j, k)}{\Delta r} \right\},
\] (5.54)

\[
C_{eth}(i, j, k) = \frac{\Delta t}{\epsilon(i, j, k)};
\]

\[
\bar{E}_{\phi}^{n+1}(i, j, k) = \frac{1}{a_{r}(i) + \frac{\Delta t \sigma_{r}(i)}{2\epsilon}} \left\{ \left( a_{r}(i) - \frac{\Delta t \sigma_{r}(i)}{2\epsilon} \right) \bar{E}_{\phi}^{n}(i, j, k) + \right.
\]

\[
C_{eph}(i, j, k) \left[ \frac{\bar{H}_{\phi}^{n+\frac{1}{2}}(i, j, k) - \bar{H}_{\phi}^{n+\frac{1}{2}}(i - 1, j, k)}{\Delta r} - \frac{1}{\Delta \theta} \left( a_{r}(i) \left[ H_{r}^{n+\frac{1}{2}}(i, j, k) - H_{r}^{n+\frac{1}{2}}(i, j - 1, k) \right] + \frac{\sigma_{r}(i)}{\epsilon} \left[ H_{rs}^{n+\frac{1}{2}}(i, j, k) - H_{rs}^{n+\frac{1}{2}}(i, j - 1, k) \right] \right) \right\},
\] (5.55)

\[
C_{eph}(i, j, k) = \frac{\Delta t}{\epsilon(i, j, k)};
\]
\begin{equation}
E_{\theta,\phi}^{n+1}(i,j,k) = \frac{1}{b_r(i)} \left[ \bar{E}_{\theta,\phi}^{n+1}(i,j,k) - (1 - e^{-\frac{\Delta t}{\Delta r_0^2(i)}})Q_{\theta,\phi}^{n+1}(i,j,k) \right], \quad (5.56)
\end{equation}

\begin{equation}
Q_{\theta,\phi}^{n+1}(i,j,k) = \bar{E}_{\theta,\phi}^{n+1}(i,j,k) + e^{-\frac{\Delta t}{\Delta r_0^2(i)}}Q_{\theta,\phi}^{n}(i,j,k), \quad (5.57)
\end{equation}

\begin{equation}
Q_{\theta,\phi}^{0}(i,j,k) = 0; \quad (5.58)
\end{equation}

and

\begin{equation}
H_{r,s}^{n+\frac{1}{2}}(i,j,k) = H_{r,s}^{n-\frac{1}{2}}(i,j,k) + \Delta t H_{r}^{n+\frac{1}{2}}(i,j,k). \quad (5.59)
\end{equation}

At each time step, we calculate the discrete summation in equation 5.59 from magnetic fields before the electric field updates in equations 5.54-5.56. This summation corresponds to the integral term in equation 5.48.

In the above equations, \(i, j, k\) and \(\Delta r, \Delta \theta, \Delta \phi\) correspond to grid cell indexes and discretization steps in radial, elevation, and azimuthal directions, respectively. FDTD time step is given \(\Delta t\). And \(i^{\pm} = i \pm 0.5\) (similarly \(j^{\pm} = j \pm 0.5\) and \(k^{\pm} = k \pm 0.5\)) depending on concerned field’s location in the Yee cell for spherical FDTD as shown in figure 5.2. The discretization is based on central differencing in both time and space.

**5.4.2 Update Sequence**

Since there are new field terms in the PML region \((E_{\theta,\phi}, \bar{E}_{\theta,\phi}, H_{\theta,\phi}, \bar{H}_{\theta,\phi})\), the question arises as to which field needs to be updated first. Moreover, because of the presence of additional field terms in stretched-coordinate formulation, field updates at the PML and non-PML interface needs to be handled carefully. Assuming the interface is at \(r = r_0\), the following update sequence for the above update equations addresses these issues.

1. **Update \(E_r\):**
   - Update \(E_r\) in inner non-PML region.
   - Update \(E_r\) in PML region using equation 5.53.
Figure 5.2: Spherical FDTD unit cell showing the field locations and their offsets.

(2) **Update** $E_\theta$:

- Update $E_\theta$ in inner non-PML region.
- Calculate $H_{rs}$ in equation 5.59 using magnetic fields.
- Calculate $\bar{H}_\phi$ near PML interface (yet, that still belongs to inner region, i.e., $r = r_0 - \frac{\Delta r}{2}$) using $\bar{H}_\phi = rH_\phi$. This is needed for $\bar{E}_\theta$ update.
- Update $\bar{E}_\theta$ in PML region using equation 5.54.
- Calculate $Q_\theta$ in PML region using equation 5.57.
- Calculate $E_\theta$ in PML region using equation 5.56.

(3) **Update** $E_\phi$:

- Calculate $\bar{H}_\theta$ near PML interface (yet, that still belongs to inner region, i.e., $r = r_0 - \frac{\Delta r}{2}$) using $\bar{H}_\theta = rH_\theta$. This is needed for $\bar{E}_\phi$ update.
- Update $\bar{E}_\phi$ in PML region using equation 5.55.
- Calculate $Q_\phi$ in PML region using equation 5.57.
- Calculate $E_\phi$ in PML region using equation 5.56.

As mentioned earlier, at the interface between the inner region and PML, the update to tangential Electric fields in equations 5.54 and 5.55 that can be considered part of PML, require magnetic fields in the inner non-PML region. To put these non-PML magnetic fields in the format of equation 5.37 as required by update equations 5.54 and 5.55 we multiply them with radius, i.e, $\vec{H}_{\theta,\phi}(\omega) = r H_{\theta,\phi}(\omega)$. It is to be noted that the radius $r$ is not a function of frequency $\omega$, as these magnetic fields are located in inner non-PML region that is not stretched.

### 5.4.3 Magnetic Field Stretched-Coordinate PML Equation

In a similar fashion to the above derivation of electric field update equations in spherical PML region, magnetic field update equation can be derived. Frequency domain Faraday’s law in complex coordinate space, stretched only along radial direction, in spherical coordinate system are given by:

\[
\begin{align*}
\jmath \omega \mu H_r(\omega) &= -\frac{1}{r \sin \theta} \left[ \frac{\partial}{\partial \theta} (\sin \theta E_\phi(\omega)) - \frac{\partial}{\partial \phi} E_\theta(\omega) \right] \quad (5.60) \\
\jmath \omega \mu H_\theta(\omega) &= -\frac{1}{r} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (E_r(\omega)) - \frac{\partial}{\partial r} (r E_\phi(\omega)) \right] \quad (5.61) \\
\jmath \omega \mu H_\phi(\omega) &= -\frac{1}{r} \left[ \frac{\partial}{\partial r} (r E_\theta(\omega)) - \frac{\partial}{\partial \theta} E_r(\omega) \right], \quad (5.62)
\end{align*}
\]

In time domain, the above equations translate to:

\[
\begin{align*}
\mu \left( b_r(r) \frac{\partial}{\partial t} + \frac{\Delta_r(r)}{\epsilon} \right) H_r(t) &= -\frac{1}{\sin \theta} \left[ \frac{\partial}{\partial \theta} (\sin \theta E_\phi(t)) - \frac{\partial}{\partial \phi} (E_\theta(t)) \right] \quad (5.63) \\
\mu \left( a_r(r) \frac{\partial}{\partial t} + \frac{\sigma_r(r)}{\epsilon} \right) \tilde{H}_\theta(t) &= -\frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (s_r(t) * E_r(t)) + \frac{\partial}{\partial r} (\tilde{E}_\phi(t)) \quad (5.64) \\
\mu \left( a_r(r) \frac{\partial}{\partial t} + \frac{\sigma_r(r)}{\epsilon} \right) \tilde{H}_\phi(t) &= -\frac{\partial}{\partial r} (\tilde{E}_\theta(t)) + \frac{\partial}{\partial \theta} (s_r(t) * E_r(t)) \quad (5.65) \\
E_{\theta,\phi}(t) &= r^{-1}(t) * \tilde{E}_{\theta,\phi}(t), \quad (5.66) \\
H_{\theta,\phi}(t) &= r^{-1}(t) * \tilde{H}_{\theta,\phi}(t). \quad (5.67)
\end{align*}
\]

Similar to Ampere’s law, the Faraday’s law’s update equations for FDTD implementation of
the time domain stretched-coordinate PML equations (5.63-5.67) are given by:

\[ H^{n+\frac{3}{2}}_r(i,j,k) = \frac{1}{b_r(i)} + \frac{\Delta t \Delta r(i)}{2 \epsilon} \left\{ \left( b_r(i) - \frac{\Delta t \Delta r(i)}{2 \epsilon} \right) H^{n-\frac{1}{2}}_r(i,j,k) + \right. \]

\[ \text{Chre}(i,j,k) \left[ - \frac{E^n_\theta(i,j+1,k) \sin((j+1)\Delta \theta) - E^n_\phi(i,j,k) \sin(j\Delta \theta)}{\Delta \theta} \right. \]

\[ + \left. \frac{E^n_\theta(i,j,k+1) - E^n_\theta(i,j,k)}{\Delta \phi} \right\}, \quad (5.68) \]

\[ Chre(i,j,k) = \frac{\Delta t \Delta \theta}{2 \sin(j+\Delta \theta) \mu(i,j,k) \sin(\frac{\Delta \theta}{2})}; \]

\[ \bar{H}^{n+\frac{1}{2}}_\theta(i,j,k) = \frac{1}{a_r(i^+) + \frac{\Delta t \sigma_r(i^+)}{2 \epsilon}} \left\{ \left( a_r(i^+) - \frac{\Delta t \sigma_r(i^+)}{2 \epsilon} \right) H^{n-\frac{1}{2}}_\theta(i,j,k) + \right. \]

\[ \text{Chte}(i,j,k) \left[ - \frac{1}{\Delta \phi \sin(j \Delta \theta)} \left( a_r(i^+) \left[ E^n_r(i,j,k+1) - E^n_r(i,j,k) \right] + \right. \right. \]

\[ \left. \left. \frac{\sigma_r(i^+)}{\epsilon} \left[ E^n_{rs}(i,j,k+1) - E^n_{rs}(i,j,k) \right] \right) \right\}. \quad (5.69) \]

\[ Chte(i,j,k) = \frac{\Delta t}{\mu(i,j,k)}; \]

\[ \bar{H}^{n+\frac{1}{2}}_\phi(i,j,k) = \frac{1}{a_r(i^+) + \frac{\Delta t \sigma_r(i^+)}{2 \epsilon}} \left\{ \left( a_r(i^+) - \frac{\Delta t \sigma_r(i^+)}{2 \epsilon} \right) H^{n-\frac{1}{2}}_\phi(i,j,k) + \right. \]

\[ \text{Chpe}(i,j,k) \left\[ - \frac{E^n_\theta(i+1,j,k) - E^n_\phi(i,j,k)}{\Delta r} \right. \]

\[ + \left. \frac{1}{\Delta \theta} \left( a_r(i^+) \left[ E^n_r(i,j,k+1) - E^n_r(i,j,k) \right] + \right. \right. \]

\[ \left. \left. \frac{\sigma_r(i^+)}{\epsilon} \left[ E^n_{rs}(i,j,k+1) - E^n_{rs}(i,j,k) \right] \right) \right\}. \quad (5.70) \]

\[ Chpe(i,j,k) = \frac{\Delta t}{\mu(i,j,k)}; \]
\[
H_{\theta,\phi}^{n+\frac{1}{2}}(i,j,k) = \frac{1}{b_r(i)} \left[ \tilde{H}_{\theta,\phi}^{n+\frac{1}{2}}(i,j,k) - (1 - e^{-\frac{\Delta t}{\gamma}(i)})R_{\theta,\phi}^{n+\frac{1}{2}}(i,j,k) \right], \tag{5.71}
\]
\[
R_{\theta,\phi}^{n+\frac{1}{2}}(i,j,k) = \tilde{H}_{\theta,\phi}^{n+\frac{1}{2}}(i,j,k) + e^{-\frac{\Delta t}{\gamma}(i)}R_{\theta,\phi}^{n}(i,j,k),
\]
\[
R_{\theta,\phi}^{\frac{3}{2}}(i,j,k) = 0;
\]
and
\[
E_{rs}^{n}(i,j,k) = E_{rs}^{n-1}(i,j,k) + \Delta t E_{r}^{n}(i,j,k). \tag{5.72}
\]

At each time step, we calculate the discrete summation in equation 5.72 from electric fields before the magnetic field updates in equations 5.69-5.71.

5.5 PML Reflection Analysis in Continuous Medium

In this section, the PML reflection coefficient is derived in continuous space. This will later act as benchmark for comparing the absorption performance of different PML and ABC formulations given above. Ideally, if the PML medium extends to infinity in continuous space, the reflection coefficient is zero. However, for practical PML implementation in methods such as FDTD, PML thickness is finite and a perfect electric conductor (PEC) wall terminates the grid as shown in figure 5.3. As shown in the figure, the PML region stretches from radius \( r_0 \) to \( r_1 \). The incident wave gets attenuated while passing through the PML, reaches the PEC wall and gets reflected. This reflected wave travels towards the inner region. Although it gets attenuated in the process again, it is of finite amplitude. Therefore, a non-zero reflected wave will appear in the inner region because of the PEC wall backing PML. The reflected wave, and by extension, the associated reflection coefficient can be mathematically derived. A similar analysis for continuous-space cylindrical PML is given in [72].

The incident wave for \( TE_r \) case (transverse electric to radial direction) in the inner region in terms of spherical elementary functions dealt in chapter 4 and \([60]\) can be written as:
\[
E_\phi^+ = -\beta \sin \theta \, h_n^{(2)}(\beta r) P_n^m(\cos \theta) e^{-j(m\phi)}, \tag{5.73}
\]
Figure 5.3: The position of PML region and PEC wall relative to origin.

where, $h_n^{(2)}(\beta r)$ represents an outward traveling wave.

Because of the stretching along the radial direction as given in equation 5.30, the incident wave in the PML region transforms to:

$$E_{\phi,PML}^+ = -\beta \sin \theta h_n^{(2)} \left( \beta (r_0 + \int_{r_0}^r s(r, \omega) \, dr') \right) P_n'(\cos \theta) e^{-j(m \phi)},$$  \hspace{1cm} (5.74)

where $r_0$ is the inner radius of the PML.

The reflected wave from the PEC backing the PML at radius $r_1$ is given by:

$$E_{\phi,PML}^- = k \cdot \beta \sin \theta h_n^{(1)} \left( \beta (r_0 + \int_{r_0}^{r_1} s(r, \omega) \, dr') \right) P_n'(\cos \theta) e^{-j(m \phi)}.$$ \hspace{1cm} (5.75)

Here, $h_n^{(1)}(\beta r)$ represents an outward traveling wave. The dimension-less constant $k$ can be found from the tangential boundary condition at the PEC as follows:

$$k = \frac{h_n^{(2)} \left( \beta (r_0 + \int_{r_0}^{r_1} s(r, \omega) \, dr') \right)}{h_n^{(1)} \left( \beta (r_0 + \int_{r_0}^{r_1} s(r, \omega) \, dr') \right)},$$ \hspace{1cm} (5.76)

where, $r_1$ is the outer radius of the PML (PEC wall).

Thus, the reflection coefficient is given by:

$$\Gamma = \frac{E_{\phi,PML}^-|_{r=r_0}}{E_{\phi,PML}^+|_{r=r_0}} = -\frac{h_n^{(2)} \left( \beta (r_0 + \int_{r_0}^{r_1} s(r, \omega) \, dr') \right)}{h_n^{(1)} \left( \beta (r_0 + \int_{r_0}^{r_1} s(r, \omega) \, dr') \right)} \cdot \frac{h_n^{(1)}(\beta r_0)}{h_n^{(2)}(\beta r_0)},$$ \hspace{1cm} (5.77)
This analytical reflection coefficient is used as benchmark for the PML/ABC formulations discussed in earlier sections for spherical FDTD, in the following section where PML performance is analyzed.

5.6 PML Performance Analysis

The formulations in the above sections (split-field PML, absorbing shell and stretched-coordinate based PML) are used to truncate a free space region in spherical FDTD, and the reflection errors are analyzed for different PML/ABC parameters. In this section, the absorption performance of these formulations are compared. The continuous-space reflection coefficient for spherical PML in equation 5.77 derived in the previous section is used as benchmark for comparison.

5.6.1 Geometric Grading of PML Parameters

For implementation of PML in an FDTD scheme (decretized space), the PML parameters such as $\sigma$ and $a$ in equation 5.31 are changed gradually from one FDTD PML cell to the next, instead of an abrupt change. This minimizes the numerical reflections [12]. These parameters’ values are changed typically from 0 (at the interface between inner region and PML region) to a maximum value just before the PEC backing. For example, these maximum values are given in the equations 5.78 as $\sigma_{max}$ and $a_{max}$. However in continuous space, even an abrupt change of the PML parameters will work (not cause any spurious reflection) as long as the impedance match condition ($\frac{\sigma}{\mu} = \frac{\sigma^*}{\mu}$) is satisfied. In the following equations, this gradual change is implemented using polynomial grading as in [12].

$$\sigma_r(r) = \sigma_{max} \left( \frac{r - r_0}{N\Delta r} \right)^{n_{\sigma}}$$  \hspace{1cm} (5.78)

$$a_r(r) = 1 + (a_{max} - 1) \left( \frac{r - r_0}{N\Delta r} \right)^{n_{a}}$$  \hspace{1cm} (5.79)

$$\Delta_r(r) = \sigma_{max} \frac{N\Delta r}{n_{\sigma} + 1} \left( \frac{r - r_0}{N\Delta r} \right)^{n_{\sigma} + 1}$$  \hspace{1cm} (5.80)
\[ b_r(r) = r + (a_{\text{max}} - 1) \frac{N \Delta r}{n_a + 1} \left( \frac{r - r_0}{N \Delta r} \right)^{n_a + 1} \] (5.81)

Here \( n_\sigma \) and \( n_a \) are the orders of grading for PML parameters \( \sigma_r \) and \( a_r \), respectively, and \( N \) is the number of PML layers. \( \sigma_{\text{max}} \) and \( a_{\text{max}} \) are the maximum values of PML parameters \( \sigma \) and \( a \) and they will reach their respective maximum values towards the end of the PML region (near the PEC wall). For example, the variation of conductivity \( \sigma_r \) in PML region for different orders \( n_\sigma \) is shown in figure 5.4.

![Figure 5.4: Variation of conductivity \( \sigma_r \) in the PML region for different orders \( n_\sigma \)](image)

### 5.6.2 Simulation Space and Parameters

This section discusses the simulation space and parameters chosen to study the PML performance. The problem space in figure 5.5 shows the positions of source and observation, and sizes of inner non-PML and outer PML regions simulation parameters are listed in table 5.1. A much larger simulation as shown in figure 5.6 is run to get the reference fields that are not contaminated by any reflection from grid truncation.

The normalized reflection error, defined as the normalized maximum difference between the fields from reference simulation (of problem space shown in figure 5.6) and from the test problem at hand (in figure 5.5), can be calculated according to the equation 5.82. This normalized error in
<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resolution</td>
<td>40 cells/wavelength at $f = 1$ GHz ($\omega = 2\pi f$)</td>
</tr>
<tr>
<td>Number of grid cells in $r, \theta, \phi$ directions</td>
<td>$(N_r, N_\theta, N_\phi) = (61, 13, 17)$. $N_r$ includes PML layers</td>
</tr>
<tr>
<td>Source Location</td>
<td>2nd cell (Solid spherical shell close to origin shown in figure 5.5)</td>
</tr>
<tr>
<td>Observation Location</td>
<td>31st cell</td>
</tr>
<tr>
<td>Number of PML Layers ($N$)</td>
<td>10</td>
</tr>
<tr>
<td>$a_{max}$</td>
<td>0</td>
</tr>
</tbody>
</table>

The discretized PML implementation is equivalent of reflection coefficient in continuous-space PML.

$$\text{Normalized Reflection Error, } dB = 20 \log \left( \frac{|E_{\phi,\text{test}} - E_{\phi,\text{ref}}|_{max}}{|E_{\phi,\text{ref}}|_{max}} \right)$$ (5.82)

Two similar yet subtly different phenomena contribute to the normalized error in discrete PML implementation:

1. reflections from PEC wall backing the PML region and,

2. reflections from layers in discretized PML because of finite change in PML parameters, given in equations 5.78-5.81 from layer to layer.
The PML parameters such as the polynomial orders $n_\sigma, n_a$ and $\sigma_{\text{max}}$ can be tweaked to minimize the reflection error caused by above phenomena as is done in Cartesian FDTD PML implementation.

5.6.3 Performance Analysis and Comparison

To begin the PML performance analysis, the split-field PML formulation for spherical FDTD given in section 5.2 and the Absorbing Shell boundary condition for spherical FDTD given in section 5.3 are implemented numerically. And, the normalized reflection error given in equation 5.82 is compared for these two formulations in figure 5.7. The figure shows how the normalized reflection error varies with maximum conductivity $\sigma_{\text{max}}$ of equation 5.78 at different elevations angles $\theta$ in the grid. Since the excitation and the problem space are spherically symmetric, it is expected that the PML performance doesn’t depend on elevation angle $\theta$ or azimuth angle $\phi$ as can be observed in the figure.

However, surprisingly, the comparison shows that the performance of about -30 dB reflection for split-field formulation in spherical FDTD is identical to that of absorbing shell boundary con-
dition. This is in contrast to less-than -50dB of reflection errors easily attainable with split-field PML formulation in Cartesian FDTD. The reason why split-field PML performance is not at par with its Cartesian coordinate counterpart is analyzed in later sections of the chapter.

Next, the stretched-coordinate PML formulation for spherical FDTD given in section 5.4 is implemented numerically for the same problem space and relevant simulation parameters as above. Figure 5.8 shows how normalized reflection error varies with respect to $\sigma_{\text{max}}$ for stretched-coordinate PML formulation. The minimum reflection error possible with stretched-coordinate PML for $n_{\sigma} = 2$ is about -80 dB when compared to -30 dB from split-field PML formulation. The figure also shows how the reflection error varies as $n_{\sigma}$ is changed.

Also, similar to Cartesian coordinate PML case, there is an optimum $\sigma_{\text{max}}$ for every $n_{\sigma}$ at which the reflection error is minimum. Below this optimum value, the reflection error quickly increases with decreasing $\sigma_{\text{max}}$. Above this optimum value, the reflection error increases albeit slowly. This is because, for the former case where $\sigma_{\text{max}}$ is low, the incident wave is not attenuated enough in PML region by the time it reaches PEC backing, where it gets reflected. While for the latter case where $\sigma_{\text{max}}$ is high, the reflections caused by the discretized PML parameters dominate.
the reflection from the PEC wall. Moreover, it is shown in figure 5.9 that in continuous PML, i.e., in the absence of discretization, the reflection error continues to decrease with increasing $\sigma_{\text{max}}$. This is because, having traveled through highly lossy medium, there is only so much incident wave amplitude left to get reflected by the PEC backing.

Figure 5.8: Comparison of Reflection Error for stretched-coordinate PML for various PML polynomial orders $n_\sigma$

Figure 5.9: Reflection Error for different mode numbers $n$ and $m = 0$ in Continuous and FDTD PML cases.
Figure 5.9 compares the reflection error from stretched-coordinate PML for spherical FDTD and the continuous-space reflection coefficient given by equation 5.77 for various mode excitations (with variable $n$ and $m = 0$). As mentioned before in table 5.1, the source is a spherical shell of radius $2\Delta r$, where $\Delta r$ is the radial discretization step. The sourcing is done by adding a time series to a field component (soft sourcing) as shown in equation 5.83 that acts as a current source. And as shown in the equation, the soft source has a $\theta$-dependent profile to excite a certain $n$ mode ($n = 1$ case is showed in the equation as an example).

$$H_r|_{q}^{n}(2,j,:) = H_r|_{q}^{n}(2,j,:) + \cos\left(\left(j \cdot \frac{1}{2}\right) \Delta \theta\right) \cdot f(q\Delta t), \quad (5.83)$$

$$f(q) = \frac{1}{32} [10 - 15 \cos(\omega q \Delta t) + 6 \cos(2\omega q \Delta t) - \cos(3\omega q \Delta t)]. \quad (5.84)$$

Here $j$ is index for elevation angle $\theta$, and $\Delta \theta$ is discretized elevation angle step. And, $f(q\Delta t)$ is the time series, here shown as Blackman-Harris waveform in equation 5.84 as an example, where $q$ represents the $q^{th}$ time step and $\Delta t$ is discretization time step of the FDTD simulation. This waveform is a periodic waveform containing pulses of period $\frac{2\pi}{\omega}$. Only one such pulse is introduced to let it propagate outward and observe it after getting reflected by PML, as in a pulsed-radar. As such, the sourcing is time-gated, i.e. introduced only in the time limits $0 < n\Delta t < \frac{2\pi}{\omega}$.

Associated Legendre functions for different $n$ are given in table 5.2 and mode $n$ can be excited in the FDTD grid by introducing respective $\theta$ profile in equation 5.83.

Table 5.2: Legendre Polynomials $P_n^m(\cos \theta)$ for some lower order $n$ and $m = 0$

<table>
<thead>
<tr>
<th>$n$</th>
<th>$P_n^0(\cos \theta)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$\cos \theta$</td>
</tr>
<tr>
<td>2</td>
<td>$\frac{1}{2}(3 \cos^2 \theta - 1)$</td>
</tr>
<tr>
<td>3</td>
<td>$\frac{1}{2} \cos \theta(5 \cos^2 \theta - 3)$</td>
</tr>
</tbody>
</table>

5.7 Why Split-Field PML doesn’t work in Spherical FDTD?

In Cartesian FDTD, the split-field PML formulation will lead to stretched-coordinate PML formulation and vice-versa as shown in the equations below. Starting with scalar Maxwell’s differ-
ential equation for \( E_y \) and its split-field notation, we arrive at the stretched-coordinate notation for \( E_y \).

\[
(j\omega + \sigma) E_y = \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} \quad (5.85)
\]

\[
j\omega \epsilon E_{yz} + \sigma_z E_{yz} = \frac{\partial H_x}{\partial z} \quad \Rightarrow \quad j\omega \epsilon E_{yz} = \frac{1}{S_z} \frac{\partial H_x}{\partial z} \quad (5.86)
\]

\[
j\omega \epsilon E_{yx} + \sigma_x E_{yx} = -\frac{\partial H_z}{\partial x} \quad \Rightarrow \quad j\omega \epsilon E_{yx} = -\frac{1}{S_x} \frac{\partial H_z}{\partial x} \quad (5.87)
\]

Adding the later parts of the above two equations we arrive at the following equation:

\[
j\omega \epsilon E_y = \frac{1}{S_z} \frac{\partial H_x}{\partial z} - \frac{1}{S_x} \frac{\partial H_z}{\partial x} \quad (5.88)
\]

Starting with Maxwell’s equations in complex stretched-coordinate space and then modifying it to include stretching variable as shown below, we arrive at equation 5.91 which is the same as equation 5.88.

\[
j\omega \epsilon E_y = \frac{\partial H_x}{\partial z} \cdot \frac{1}{S_z} \frac{\partial H_z}{\partial x} \quad (5.89)
\]

\[
\frac{\partial}{\partial \tilde{x}} = \frac{1}{S_x} \frac{\partial}{\partial x}, \quad \frac{\partial}{\partial \tilde{z}} = \frac{1}{S_z} \frac{\partial}{\partial z} \quad (5.90)
\]

\[
j\omega \epsilon E_y = \frac{1}{S_z} \frac{\partial H_x}{\partial z} - \frac{1}{S_x} \frac{\partial H_z}{\partial x} \quad (5.91)
\]

where,

\[
S_{x,z} = \left( 1 + \frac{\sigma_{x,z}}{j\omega \epsilon} \right),
\]

\[
\tilde{x} = \int_{x=0}^{x'} S_x(x') \, dx', \text{ and}
\]

\[
\tilde{y} = \int_{y=0}^{y'} S_y(y') \, dy'.
\]

Therefore, split-field and stretched-coordinate PML formulation in Cartesian coordinates are identical although their interpretation and mathematical representations are different.

On the other hand for the PML in spherical FDTD, however, the split-field and stretched-coordinate formulations do not lead to one another as shown below. Starting with split-field equations 5.7 and 5.8 for \( E_\theta \), and using the stretched-coordinates variable \( s_r \), we get the field
equation for $E_{\theta}$ in stretched-coordinates as shown in equation 5.98 following the process below.

$$j\omega \epsilon E_{\theta\phi} = \frac{1}{r} \frac{\partial H_r}{\partial \phi}$$ (5.92)

$$j\omega \left( 1 + \frac{\sigma_r}{j\omega} \right) E_{\theta r} = -\frac{1}{r} \frac{\partial (r H_\phi)}{\partial r}$$ (5.93)

$$s_r = \left( 1 + \frac{\sigma_r (r)}{j\omega \epsilon} \right)$$ (5.94)

$$j\omega \epsilon E_{\theta r} = -\frac{1}{s_r r} \frac{\partial (r H_\phi)}{\partial r}$$ (5.95)

$$j\omega \epsilon E_{\theta\phi} = \frac{1}{r} \frac{\partial H_r}{\partial \phi}$$ (5.96)

$$j\omega \epsilon E_{\theta} = \frac{1}{r \sin \theta} \frac{\partial (s_r \cdot H_r)}{\partial \phi} - \frac{1}{s_r r} \frac{\partial (r H_\phi)}{\partial r}$$ (5.97)

$$j\omega \epsilon S_r \bar{r} E_{\theta} = \frac{1}{\sin \theta} \frac{\partial (S_r \cdot H_r)}{\partial \phi} - \frac{\partial (\bar{r} H_\phi)}{\partial r}$$ (5.98)

Whereas, if we start with Maxwell’s equation in complex stretched-coordinate space as in equation 5.28 repeated here in equation 5.99 and modify it by introducing stretched-coordinate variable $S_r$, we arrive at equation 5.102. This is essentially different from equation 5.98 that we arrived at from the split-field formulation in the sense that radius $r$ in equation 5.98 is real whereas the $\bar{r}$ in equation 5.102 is a complex (frequency dependent) stretched-coordinate radius.

$$j\omega \epsilon E_{\theta}(\omega) = \frac{1}{\bar{r}} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (H_r(\omega)) - \frac{\partial}{\partial \bar{r}} (\bar{r} H_\phi(\omega)) \right]$$ (5.99)

$$\frac{\partial}{\partial \bar{r}} = \frac{1}{S_r} \frac{\partial}{\partial r}$$ (5.100)

$$j\omega \epsilon E_{\theta}(\omega) = \frac{1}{\bar{r}} \left[ \frac{1}{\sin \theta} \frac{\partial}{\partial \phi} (H_r(\omega)) - \frac{\partial}{\partial S_r \partial r} (\bar{r} H_\phi(\omega)) \right]$$ (5.101)

$$j\omega \epsilon S_r \bar{r} E_{\theta} = \frac{1}{\sin \theta} \frac{\partial (S_r \cdot H_r)}{\partial \phi} - \frac{\partial (\bar{r} H_\phi)}{\partial r}$$ (5.102)

Thus, the split-field PML formulation for spherical FDTD doesn’t truly reflect the complex stretched-coordinates as it does for the Cartesian case.
Chapter 6

Conclusion

This thesis introduced some advanced formulations and applications of finite difference time domain method while reviewing the existing methods.

The second chapter dealt with the development of a plane wave excitation formulation for FV24, a finite-volume based higher-order FDTD variant. Now that the leakage-free and efficient plane wave excitation method is available for FV24, and owing to its excellent phase error characteristics, FV24 can be applied to electrically large problems such as a ship or an aircraft for studying their scattering cross section, or for understanding propagation of mobile radio waves in urban setting etc.

The plane wave excitation method based on total field/scattered field formulation and Discrete planewave technique is reviewed for conventional FDTD before implementing it for FV24. In the process, the concept of auxiliary 1D grid is elucidated clearly by showing its relation to the main FDTD 3D grid. First, it is represented as an imaginary line along the direction of propagation of plane wave. Then, the electric and magnetic field locations of the main grid are projected on to this imaginary line forming the auxiliary 1D grid. It is shown that the 1D grid has co-located electric fields separately from co-located magnetic fields. Multiple electric field locations (or magnetic field locations) on the main 3D grid will have projection at the same location on the 1D grid. This visual demonstration of the 1D grid and its properties, absent in the literature, will greatly help in understanding the technique. Subsequently, the indexing for 1D update equations which help propagate plane along the 1D auxiliary grid is demonstrated. It is pointed out why such a 1D grid
will have the same dispersion relation as that of the main 3D grid.

Since FV24 computational stencil extends multiple Yee cells, the consistency corrections needed to implement TF/SF formulation become complex and confusing, especially at the edges and corners of the TF/SF interface. Hence the consistency corrections are dealt with systematically and visually shown to aid easy understanding and replication. Initiation of the plane wave on the auxiliary 1D grid by hard sourcing initial grid points is equally complex for FV24 given its extended stencil. It is also well explained to avoid any pitfalls. Finally, the leakage free plane wave excitation is demonstrated. The spurious leakage into the scattered field is below -300 dB that is same as the noise floor set by the machine precision. It is made possible because of the numerical dispersion match between the auxiliary 1D and the 3D grids.

In the later parts of this chapter, different near to farfield transformation approaches possible in FDTD are compared for accuracy. The spatial interpolation of fields is required in FDTD to calculate fictitious currents on the equivalent surface, that in turn are used to calculate farfields. Different interpolation techniques such as the arithmetic averaging, geometric mean, Mixed-surface, and separate-surface approaches are possible. The performance of these different interpolations in estimating the farfields is compared. The empty scatterer case that ideally produces zero farfield sets the baseline and is selected to compare the performance of above interpolation schemes. It is shown that the arithmetic averaging and Mixed-surface interpolation schemes perform better than the other two. It is also validated by calculating the radar cross-section of a canonical dielectric cube using different FDTD interpolation techniques and comparing them with commercial solvers such as FEKO and HFSS.

Therefore, we can combine the plane wave excitation method for FV24 dealt here and the Mixed-surface or arithmetic averaging approach for performing near to farfield transformation, to analyze radar cross section or radiation pattern of electrically large structures accurately.

The third chapter deals with application of FDTD to an interesting problem encountered in printed circuit boards. The composition of composite dielectric materials used in PCBs, and the root cause of the glass weave-induced skew are reviewed first. Then it is noted that the glass weave-
induced skew in a differential transmission line can cause a variety of problems such as increased bit error rates affecting the robustness of the digital system, and increased radiated emissions causing compliance failures. This research applies auxiliary differential equation (ADE) formulation for FDTD, that helps model frequency dependence of material properties of real materials, to estimate glass weave-induced skew in a differential pair.

The implementation of ADE method is demonstrated using multi-pole Debye model. At first, the broadband profile of real and imaginary parts of complex permittivity are obtained using Djordjevic-Sarkar model using minimal input data points. Real and imaginary parts at just a single frequency point often suffice to generate broadband profiles. Then the broadband Debye coefficients are obtained by fitting multi-pole Debye model to Djordjevic-Sarkar model. The FDTD update equations are subsequently modified to account for the multi-pole Debye model.

The geometric model of glass weave is implemented mathematically and the FDTD cells in the grid are assigned different materials such as glass, resin, PEC (for microstrip traces), and free space. This segregates the dispersive-material cells from the non-dispersive cells. The update equations at the dispersive cells are modified to include the multi-pole Debye model using the ADE formulation. The glass-weave induced skew is calculated for a sample differential pair and validated with the results from HFSS. Also, the performance in terms of memory and time consumption are compared. The advantages of using FDTD method for glass weave skew study are elucidated. Finally, the use of graphical processing units (GPUs) to accelerate the skew simulations in MATA LB is demonstrated.

The fourth chapter deals with the derivation of numerical dispersion relation for spherical FDTD, sensitivity study of the associated numerical wave number, and the stability analysis of spherical FDTD. At first, the structure of spherical grid, field locations, and update equations are reviewed. The non-uniformity of spherical grid is visualized particularly near the origin. The numerical dispersion relation for Cartesian FDTD is reviewed initially. Later, the derivation process is generalized and applied to spherical FDTD.

The electric and magnetic fields are first given in terms of the elementary functions native to spherical coordinate system. Then, they are substituted in spherical FDTD update equations.
Finally, the resultant equations are reduced to obtain the numerical dispersion relation. The numerical dispersion relationship thus obtained is position dependent demonstrating the non uniform nature of the spherical FDTD grid.

This numerical dispersion relation is solved using MATLAB to obtain the complex numerical wave number. It is observed that as we move close to the origin, the numerical wave number deviates from that of the free space wave number. This signifies that the wave propagation in the spherical FDTD grid is affected. To model the wave behavior at the origin with required accuracy, the grid parameters such as resolution and time step need to be chosen with care. As we move away from the origin, the numerical wave number converges to the free space wave number.

Later, the sensitivity of the numerical wave number to various grid parameters such as resolution, elevation angle and mode numbers is studied. In the later part of the chapter, an attempt is made to derive the stability criterion for the spherical FDTD grid based on the position dependent numerical dispersion relation derived earlier in the chapter. The stability criterion available in the literature are reviewed in the current study and the challenges faced during the validation of the stability criterion are documented.

The last chapter deals with the implementation of the perfectly matched layer in spherical FDTD. Firstly, the split-field formulation and the associated update equations are elucidated. Secondly, the stretched-coordinates formulation and the associated update equations are derived. Finally, an absorbing boundary condition based on lossy dielectric and the associated update equations are obtained. The effectiveness of the above three formulations in absorbing the waves in spherical FDTD is compared. It is observed that the split-field formulation performs only as good as the lossy dielectric-based absorbing boundary condition, while the stretched-coordinates formulation performs better than the rest of the two. This is in contrast to the Cartesian coordinate PML, where both the split-field and stretched-coordinates formulation perform identically.

The reflection coefficient of the continuous space PML backed by a PEC is derived and is used as a benchmark for the above formulations. It is observed that the performance of stretched-coordinates PML implemented for spherical FDTD compares well with that of the continuous space
spherical PML until the numerical errors in spherical FDTD start to degrade the performance of the spherical FDTD PML.

In the final section of the chapter, it is shown that the split-field formulation and the stretched-coordinate formulation of the PML in spherical FDTD are not identical, whereas in Cartesian coordinated system they are identical. This explains the reason, why the split-field PML formulation in spherical FDTD is not as effective in absorbing the incident waves as in Cartesian coordinate system.

6.1 Original Contributions

The original contribution of the dissertation work are:

- The plane wave excitation technique for FV24, a finite-volumes based higher order FDTD, based on total field/scattered field (TF/SF) formulation and Discrete plane wave formulation. Associated 1D grid update equations, TF/SF consistency corrections, wave initialization technique on the 1D grid and mapping of 1D grid locations to the 3D grid location and vice-versa for FV24.

- The visualization of auxiliary 1D grid, used in the above technique, as a set of projections of electric and magnetic field locations on the main grid.

- Technique for comparing the accuracy of various field interpolations techniques available in the literature that are used in the implementation of near to farfield transformation in FDTD, and its implementation.

- Technique to obtain glass weave-induced skew using FDTD by combining the implementation of glass weave structure and dispersive material characterization using auxiliary differential equation method for multi-pole Debye model. The multi-pole Debye coefficients needed for dielectric materials are obtained by curve-fitting it to Djordjevic-Sarkar model.
• Technique to compare glass weave-induced skew extracted from S-parameters obtained from HFSS simulations, and that obtained from FDTD. The same Gaussian pulse that is used as excitation in FDTD is used to window the S-parameters from HFSS and then the pulse response is calculated from inverse Fourier transforming the windowed S-parameters.

• Visualization of spherical FDTD grid and various special cells near poles and origin.

• Derivation of numerical dispersion relation in spherical FDTD for $TM_r$ modes.

• Method to observe stability criterion for spherical FDTD at different distances from origin by making the cells close to the origin as part of PEC.

• Derivation of central difference update equations based on stretched-coordinate PML formulation for spherical FDTD.

• Technique to excite various modes in spherical FDTD grid.

• Comparison of effectiveness of stretched-coordinate based PML, lossy dielectric-based absorbing shell, and split-field PML formulations for spherical FDTD.

• Derivation of continuous-space reflection coefficient of spherical PML as a benchmark for comparing performance of various truncation techniques for spherical FDTD.

• Derivation that shows split-field and stretched-coordinate PML formulations in spherical coordinates are not identical.
Bibliography


