TIME-DOMAIN SOLVERS FOR COMPLEX-MEDIA ELECTRODYNAMICS AND PLASMA PHYSICS

DISSERTATION

Presented in Partial Fulfillment of the Requirements for the Degree Doctor of Philosophy in the Graduate School of The Ohio State University

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2008

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Part of figures and text in this dissertation has appeared in the following publications (used with permission)


ABSTRACT

In this dissertation, several extensions for two popular electromagnetic simulation methods: finite-different time-domain (FDTD) and finite-element time-domain (FETD), are presented. These extensions aim to increase the geometrical flexibility and modeling capabilities in simulation of Maxwell’s equations. Since straight-forward extensions to these methods produce numerical artifacts that pollute the results and reduce accuracy, alternative strategies have been sought. Various methodologies are explored here to address these issues: A $E$-$B$ mixed-vector FETD implementation based on first order Maxwell equations is introduced. In this method a mix of electric and magnetic field variables are used, where an edge element expansion is used for the electric field and face element expansion is used for the magnetic field. Compared to the standard FETD methods, it can produce several advantages without any significant computational drawback: (i) it eliminates the spurious linear growth in time that may exist in the standard schemes; (ii) it produces energy-conserving schemes under appropriate time-discretization; (iii) it can be easily extended to frequency-dispersive media; (iv) it provides a natural path for hybridization with FDTD. Exploiting item (iii), $E$-$B$ mixed-vector FETD is extended to inhomogeneous doubly-dispersive media. A conformal-PML implementation is also proposed for efficient simulation of open-domain boundaries by significantly reducing the buffer regions in the computational domain. Despite the advantages, finite-element simulations require solution of
a linear system of equations which, in most practical problems, highly computationally intense. A hybrid FDTD-FETD method is introduced to alleviate this issue. The hybridization can result in significant optimization in computational cost by assigning detailed portion of the computational domain to FETD, while assigning the remaining to FDTD. Finally, a subgridding by domain-overriding (SGDO) methodology for full electromagnetic particle-in-cell (PIC) simulations is presented. Combined with relaxation methods, SGDO can produce significant improvements in PIC simulation accuracy.
This work is dedicated to İdil
ACKNOWLEDGMENTS

I would like to express my sincere gratitude to my advisor Professor Fernando L. Teixeira for his guidance and invaluable advices that he has given me during my studies. His commitment to his students, his passion in the subject of electromagnetics and his patience will always inspire me. I thank Professor Robert Lee and Professor Jin-Fa Lee for kindly serving as committee members in my candidacy examination and dissertation, and for all the invaluable knowledge they have passed on through their graduate level courses. I would like to thank Ryan Chilton for the discussions and all the valuable knowledge that he has shared with me. Finally I thank everyone in the Electroscience Laboratory for making all these years a great experience.
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# TABLE OF CONTENTS

<table>
<thead>
<tr>
<th>Chapter</th>
<th>Title</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Introduction</td>
<td>1</td>
</tr>
<tr>
<td>2</td>
<td>Mixed vector $E$-$B$ FETD</td>
<td>5</td>
</tr>
<tr>
<td>2.1</td>
<td>Homogeneous media</td>
<td>8</td>
</tr>
<tr>
<td>2.1.1</td>
<td>Three-dimensional case</td>
<td>8</td>
</tr>
<tr>
<td>2.1.2</td>
<td>Two-dimensional $\text{TE}_2$ and $\text{TM}_2$ cases</td>
<td>10</td>
</tr>
<tr>
<td>2.2</td>
<td>Inhomogeneous and doubly-dispersive media</td>
<td>10</td>
</tr>
<tr>
<td>2.2.1</td>
<td>Formulation</td>
<td>10</td>
</tr>
<tr>
<td>2.2.2</td>
<td>Electric field constitutive equation update</td>
<td>11</td>
</tr>
<tr>
<td>2.2.3</td>
<td>Magnetic field constitutive equation update</td>
<td>15</td>
</tr>
<tr>
<td>2.2.4</td>
<td>Curl equations and complete update</td>
<td>16</td>
</tr>
<tr>
<td>2.3</td>
<td>Perfectly Matched Layers</td>
<td>17</td>
</tr>
<tr>
<td>2.4</td>
<td>Numerical results</td>
<td>18</td>
</tr>
<tr>
<td>2.4.1</td>
<td>Validation: Cylindrical scatterer</td>
<td>18</td>
</tr>
<tr>
<td>2.4.2</td>
<td>Perfectly matched layer performance</td>
<td>21</td>
</tr>
<tr>
<td>2.4.3</td>
<td>Zero-index lens</td>
<td>25</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
<td>Page</td>
</tr>
<tr>
<td>---------</td>
<td>----------------------------------------------------------------------</td>
<td>------</td>
</tr>
<tr>
<td>2.4.4</td>
<td>Metamaterial blueprints for reflectionless waveguide bends</td>
<td>27</td>
</tr>
<tr>
<td>2.5</td>
<td>Stability in inhomogeneous media</td>
<td>30</td>
</tr>
<tr>
<td>2.5.1</td>
<td>System matrix for discrete update equations</td>
<td>31</td>
</tr>
<tr>
<td>2.5.2</td>
<td>System matrix for semi-discrete update equations</td>
<td>32</td>
</tr>
<tr>
<td>2.5.3</td>
<td>Stability criterion</td>
<td>32</td>
</tr>
<tr>
<td>2.6</td>
<td>Late-time stability and energy conservation</td>
<td>35</td>
</tr>
<tr>
<td>2.7</td>
<td>Concluding remarks</td>
<td>36</td>
</tr>
<tr>
<td>3.1</td>
<td>Conformal PML for E-B mixed vector FETD</td>
<td>39</td>
</tr>
<tr>
<td>3.1.1</td>
<td>Electric field update</td>
<td>41</td>
</tr>
<tr>
<td>3.1.2</td>
<td>Magnetic field update</td>
<td>42</td>
</tr>
<tr>
<td>3.1.3</td>
<td>Curl equations and full update</td>
<td>45</td>
</tr>
<tr>
<td>3.2</td>
<td>Results</td>
<td>46</td>
</tr>
<tr>
<td>3.2.1</td>
<td>Scattering from a PEC circular cylinder</td>
<td>47</td>
</tr>
<tr>
<td>3.2.2</td>
<td>Conformal PML: Reflection error</td>
<td>48</td>
</tr>
<tr>
<td>3.2.3</td>
<td>Conformal PML: Parameter study</td>
<td>52</td>
</tr>
<tr>
<td>3.2.4</td>
<td>Scattering from oval PEC coated with metamaterial</td>
<td>57</td>
</tr>
<tr>
<td>3.2.5</td>
<td>Monostatic-RCS: Ogive cylinder</td>
<td>57</td>
</tr>
<tr>
<td>3.2.6</td>
<td>Late-time stability and energy conservation</td>
<td>60</td>
</tr>
<tr>
<td>3.3</td>
<td>Concluding remarks</td>
<td>64</td>
</tr>
<tr>
<td>4.1</td>
<td>General formulation</td>
<td>65</td>
</tr>
<tr>
<td>4.2</td>
<td>Finite-element update</td>
<td>67</td>
</tr>
<tr>
<td>4.2.1</td>
<td>Electric field constitutive equation update</td>
<td>68</td>
</tr>
<tr>
<td>4.2.2</td>
<td>Magnetic field constitutive equation update</td>
<td>69</td>
</tr>
<tr>
<td>4.3</td>
<td>Finite-difference update</td>
<td>72</td>
</tr>
<tr>
<td>4.4</td>
<td>Numerical results</td>
<td>73</td>
</tr>
<tr>
<td>4.4.1</td>
<td>Validation: Cylindrical scatterer</td>
<td>73</td>
</tr>
<tr>
<td>4.4.2</td>
<td>Residual error</td>
<td>74</td>
</tr>
<tr>
<td>4.4.3</td>
<td>Material traverse hybrid interface</td>
<td>80</td>
</tr>
<tr>
<td>4.4.4</td>
<td>Stability tests in free-space</td>
<td>81</td>
</tr>
<tr>
<td>4.4.5</td>
<td>PML performance</td>
<td>83</td>
</tr>
<tr>
<td>4.5</td>
<td>Concluding remarks</td>
<td>88</td>
</tr>
<tr>
<td>5.1</td>
<td>Full-electromagnetic PIC method on multi-grid components</td>
<td>89</td>
</tr>
<tr>
<td>5.1</td>
<td>Particle-In-Cell (PIC) Method</td>
<td>91</td>
</tr>
</tbody>
</table>
5.1.1 PIC Update Equations ........................................... 93
5.1.2 Solution of kinematic equations ............................... 94
5.1.3 Particle shape factor ............................................ 95
5.1.4 Gather operation ............................................... 96
5.1.5 Scatter operation ............................................... 96
5.2 Particle-in-cell implementation in subgrids....................... 101
   5.2.1 Subgridding problems in PIC ................................. 102
   5.2.2 Problems associated with interfacing electromagnetic fields. 102
   5.2.3 Problems associated with current deposition .................. 103
5.3 Numerical results ................................................ 110
   5.3.1 Verification: Gather ....................................... 111
   5.3.2 Verification: Scatter ....................................... 111
   5.3.3 Marder-Langdon relaxation convergence .................... 113
   5.3.4 Verification: Accuracy .................................... 117
   5.3.5 Laser-foil interaction .................................... 119
5.4 Concluding remarks ............................................. 121
6. Conclusions ....................................................... 122

Appendices:

A. Constants Used in Solving Dispersive Relation .................. 125

B. Layout generation algorithm for SGDO ............................ 127

Bibliography .......................................................... 134

xii
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.1</td>
<td>Permittivity values associated with the two parent faces of a given edge $j$. Note that the labeling order of faces is arbitrary.</td>
<td>13</td>
</tr>
<tr>
<td>2.2</td>
<td>Finite-element mesh for the dispersive cylindrical scatterer. The source location is indicated by the $+$ and the probe location by the $\times$.</td>
<td>20</td>
</tr>
<tr>
<td>2.3</td>
<td>Calculated field and normalized residual error produced by the mixed finite element time-domain (FETD) and finite-difference time-domain (FDTD) methods for the San Antonio clay loam cylinder model. The peak residual error of FETD is about $-50$ dB.</td>
<td>22</td>
</tr>
<tr>
<td>2.4</td>
<td>Calculated field and normalized residual error produced by the mixed finite element time-domain (FETD) and finite-difference time-domain (FDTD) methods for the doubly-dispersive cylinder model. The peak residual error of FETD method is about $-54$ dB.</td>
<td>23</td>
</tr>
<tr>
<td>2.5</td>
<td>Perfectly matched layer (PML) numerical reflection coefficient for various number of layer cells. A reflection level no larger than $-55$ dB is obtained for 8 layers for the source excitation considered.</td>
<td>24</td>
</tr>
<tr>
<td>2.6</td>
<td>Snapshot of the magnetic field at $t = 8.8151 \times 10^{-10}$ s for the zero-index lens problem. The lens is made of a homogeneous doubly-dispersive material. The field originating from a point source is refocused below the lens, demonstrating a wavefront reshaping property of this lens.</td>
<td>26</td>
</tr>
<tr>
<td>2.7</td>
<td>Cross-section of the parallel-plate waveguide in the original (bent) and transformed (straight) coordinate systems.</td>
<td>28</td>
</tr>
</tbody>
</table>
2.8 Total (main plot) and reflected (inset in dB scale) fields in the bend waveguide. The results without coarsening (about 8000 elements) do not appear in the inset plots because the reflection levels are well below $-70$ dB.

2.9 Discrete energy as a function of time inside a rectangular cavity, showing that the algorithm is energy-conserving. The inset shows the normalized magnetic field at the probe location for two different scenarios: (a) air-filled cavity (no energy dissipation) and (b) cavity filled by (lossy) dispersive and backed by a perfectly matched layer. The increase in the ripple frequency seen at late times is an artifact stemming from the log scale used for the time steps.

3.1 A conformal PML (left) can greatly reduce the amount of buffer space around the scatterer compared to the Cartesian PML (right).

3.2 Conformal PML geometry and parametrization. The point $\mathbf{r}$ along the radial direction inside the PML is given in terms of the local coordinate $\rho$ as $\mathbf{r} = \rho \hat{\rho} = (\rho_0 + l) \hat{\rho}$, as illustrated. Note that the coordinate system depicted here is a local one, with the (local) radius of curvature $\rho_0$ at the free-space/PML boundary being a function of the point M along the PML interface [99].

3.3 Scattered field and normalized residual error for a point source illuminating a circular PEC cylinder. (a) The finite element mesh comprises 33,487 edges and 22,046 faces. The source and the probe location are located at the right of the scatterer, indicated by small + and $\times$ symbols, respectively. (b) The time-domain response of the conformal PML-FETD method and the FDTD method agree very well with the analytical result. (c) Due to staircasing approximations, the error in the FDTD result is on average about 10 dB larger than the error in the FETD result for the mesh considered.

3.4 Reflection error vs. (a) time and (b) position along the PML boundary, for various $N_{PML}$: (a) The PML reflection levels are progressively reduced for larger $N_{PML}$, with $R = -68$ dB obtained for $N_{PML} = 24$. (b) The PML reflection errors peak at $90^\circ$, where the radius of curvature is minimum because a smaller radius reduces the average distance of nearby PML boundary points to the probe location. The finite-element mesh used in this example has 12,748 edges and 8,428 faces.
3.5 Reflection Error in time at location A and B \((N_{pml} = 12, \sigma_{max} = 0.5\sigma_{opt}, M = 2)\). .......................................................... 54

3.6 Reflection error at locations A and B with respect to normalized maximum conductivity and PML grading polynomial coefficient \((N_{pml} = 16)\). Optimum maximum conductivity is observed to be half of FDTD optimum value, \(\sigma_{opt}\). .......................................................... 55

3.7 Reflection error at locations A and B with respect to number of layers and the PML grading polynomial coefficient \((\sigma_{max}/\sigma_{opt} = 0.5)\). .... 56

3.8 (a) Finite element mesh for an oval-shaped PEC scatterer coated with a doubly-dispersive material. The mesh has 28,556 edges and 18,741 faces. The source and the probe are located at the right of the scatterer and indicated by small + and \(\times\) symbols, respectively. A Cartesian PML implementation for this problem would require a mesh about 1.9 times larger. (b) Scattered fields calculated by FETD and FDTD, showing very good agreement. ....................... 58

3.9 (a) The finite element mesh used to calculate the monostatic RCS of the ogive cylinder has 103,367 edges and 67,881 faces. A Cartesian PML implementation for this problem would require a mesh about 2.3 times larger. (b) Monostatic RCS of the ogive with size \(4\lambda_0 \times 1\lambda_0\) calculated by FETD, frequency-domain finite elements, and method of moments (MoM) [109]. ....................... 61

3.10 The main plot shows the discrete energy for \(10^7\) time steps inside an oval shaped cavity terminated by PEC. The energy is constant except for small periodic fluctuations due to the leap-frog approximation in the time integration. This shows the energy-conserving property of the proposed method. The inset shows the normalized magnetic field magnitude in the PEC- and PML-backed cavity simulations, showing the late-time stability of the PML. ................................. 63

4.1 Meshes used in the Hybrid FETD-FDTD simulations. Number of rectangular (\(\Box\)) and triangular (\(\triangle\)) elements used are indicated in captions of subfigures. ................................. 76
4.2 (a) Transmitted fields inside a cylindrical scatterer for different methods that are illustrated in Fig. 4.1. (b) Normalized residual error in the transmitted fields. Hybrid method accuracy matches similar methods with less number of triangular elements and thus with a smaller matrix problem to solve at each time-step. FDTD produces larger errors mainly due to geometrical modeling errors although three times higher resolution is used.

4.3 Magnetic fields and normalized residual errors for the transient response of a point source in a 3-D cubical cavity problem. Initial error level of -45 dB is obtained in both problems. The increase and decrease of the error levels in (a) and (b) in later time steps can be attributed to numerical dispersion and losses, respectively. Hybrid method produces 8 dB larger errors when compared to mixed-element FETD, due to higher numerical dispersion errors in the FDTD portion of the grid.

4.4 Residual error in transmitted field for a problem with planar hybrid interface for different resolution values. Error can be reduced down to -57 dB for \( l_e = 0.005 = \lambda_0/80 \).

4.5 Transmitted magnetic fields at the probe location for a cavity partially filled with doubly-dispersive material. Hybrid interface traversing the material interface does not introduce any significant discrepancies.

4.6 Eigenvalues of the system matrix for the mixed-FETD and hybrid FDTD-FETD methods in 2-D. The mesh used in both methods is shown in inset of (a). The mesh consists of 237 nodes, 520 edges and 284 faces. Eigenvalues are on the unit circle with the maximum discrepancy in the order of numerical noise, \( \delta < -280 \text{ dB} \). Eigenvectors associated with multiple-eigenvalues are found linearly independent.

4.7 Eigenvalues of the system matrix for the mixed-FETD and hybrid FDTD-FETD methods in 3-D. The cross-section of the mesh used in both methods is shown in inset of (a). The mesh consists of 530 nodes, 1425 edges, 1338 faces and 424 cells. Eigenvalues are on the unit circle with the maximum discrepancy in the order of numerical noise, \( \delta < -280 \text{ dB} \). Eigenvectors associated with multiple-eigenvalues are found linearly independent.
4.8 Normalized reflection error in $H_z$ for the hybrid FDTD-FETD and mixed-element FETD methods, for different number of PML. Reflection error levels of -54 dB and -79 dB are obtained in mixed-element FETD and hybrid FDTD-FETD methods, respectively. Hybrid method results in much lower PML reflections mainly due to the fact that FDTD exhibits twice the number of profile steps that exists in FETD.

5.1 Multiple solutions can be obtained for current distribution $\vec{J}$ that satisfy the discrete continuity equation for a particular charge density, $\rho$. Therefore with discrete continuity equation per se, solution for $\vec{J}$ is under-constrained. Although not trivial, additional constraints follow from the assumptions that have been already made in discretization of the kinematics updates. In the figure circles (◦) show the location of charge and charge density components, and arrows (↑) show the location of current components. Components that are colored in black have values as indicated in the figure, and all other components are zero.

5.2 Auxiliary variables $W_x$, $W_y$, and $W_z$ as sums of shifted form-factors $S$.

5.3 (a)-(d) Stuck charges that occur in an implementation where a continuity conserving algorithm is used to deposit currents onto individual grids. Stuck charge in coarse occurs since the charge is not carried further from the interface. Stuck charge with opposite sign in fine occurs since currents are withdrawn from a node that contains no charges (b). Both of these stuck charges establish static electric fields with signs that are opposite of each other. These static fields cancel out with the exception of a residue which depends on the difference in the numerical characteristic of both grids. As an example, in a case where both grids have the same resolution, static fields of these charges perfectly cancel each other without leaving any residue in electric fields.

5.4 Projectile of the particle under constant magnetic field. The magnitude of the magnetic field which is set to $B_z = 1.42 \times 10^{-4}$ successfully produces the anticipated radius of 8 m for the particle velocity $1 \times 10^8$ m/s.

5.5 Velocity of the particle as it traverses the circular path. It is found constant up to the numerical noise level.
5.6 Conservation of continuity is verified by comparing the $\nabla \cdot \vec{J}$ value obtained from the simulation with the charge density separately obtained by evaluating Eq. (5.37) separately. (e) and (f) shows a wider stencil for the current where the extra component is due to the non-trivial compensation into the old cell as the particle switches cells.

5.7 Normalized average spatial error with respect to number of iterations for different values of the correction coefficient $d = d_s/d_{\text{max}}$. Higher convergence is observed for higher $d$ values. A convergence rate of 10 dB per 105 iterations is observed for $d = 1$.

5.8 Electric fields at time step $T_{\text{max}} = 108$ for different scenarios. Spurious fields are observed in no-correction, full-domain and interface-only simulations. All-coarse field values are unresolved. toward-PML implementation can successfully simulate this problem.

5.9 Electric field and electron energy for the 1D laser-plasma interaction problem. Fine and coarse grid interface is indicated in the figure as the dotted line. Subgridding with domain-overriding shows significant improvements when compared to other methods. Significant artifacts are observed at the interface for contour- and mixed-integration.

B.1 (a) shows the grid layout in a 3D subgridding with domain-overriding problem. Individual grids are highlighted in (b),(c),(d) and (e). The conductivity scaling of PML is also illustrated in the figures.

B.2 A 2D SGDO implementation with a two-dimensional split.

B.3 SGDO subgrids created by the recursive grid generation algorithm for a 2D case for a $2 \times 2$ tile of Fig. B.2. All grid tiles except the bottom tile are coarse domains. A magnetic field snapshot is placed on top of the grids. Location of the line-source can be seen in the lower corner as a white point. An ultra-wide-band Blackmann-Harris pulse source excitation is used. The physical domains are seen as large square regions at the bottom of the grid stack, whereas the smaller auxiliary SGDO regions are on higher stacks.

B.4 Normalized residual error at the probe location for the half-space problem.
CHAPTER 1

INTRODUCTION

Finite-difference time-domain (FDTD) [1] and finite-element time-domain (FETD) [2, 3] methods are widely used electromagnetic simulation methods. They aim at simulating interactions of electromagnetic waves with underlying materials by solving Maxwell’s equations. Since these methods provide time-domain solutions for the field values, they are especially useful, but not limited, to ultra-wide-band problems such as propagation of pulses, etc. Many applications in different sub-disciplines of electrical engineering take advantage of these simulations, including: microwave and optical devices, wireless communications, electromagnetic compatibility, analysis of periodic structures and modeling of antennas. These methods have also been used in studying interactions of electromagnetic fields with charged particles. Specifically, full electromagnetic particle-in-cell (PIC) method features an extended version of the FDTD update equations and particle kinematics [4, 5].

Although both FDTD and FETD can provide accurate solutions to problems with arbitrary geometries, they are also known to possess several difficulties in implementation and performance. The inherent rectangular structure of the FDTD grid for example, considerably reduces the geometrical modeling capability. This may result
in low accuracy or computational efficiency, especially in problems with curved boundaries. Although FETD can offer accurate solutions for such problems, it is also known to possess several difficulties in implementation and performance for straightforward implementations. Some of the difficulties that are addressed in this dissertation are as follows: For FETD simulations based on the second order wave equation, spurious linear growth may be observed due to presence of spurious temporal modes. These modes exist in the null-space of the problem and they may be excited depending on the numerical characteristics of the solution method used for the matrix equation. Furthermore, implementation of doubly-dispersive materials in standard FETD is difficult due to coupling of material tensors with the wave equation. Finally, since finite-element solution requires solution of a linear system of equations in general, it is highly computationally intensive for large problems. In this dissertation several different methodologies to alleviate these problems are explored. The organization is provided below.

In Chapter 2, a $E-B$ mixed vector FETD scheme based on first order coupled Maxwell’s equations is presented. This scheme has several advantages when compared to FETD methods based on wave equations [2, 3], without any significant drawback. Some of its advantages are: (i) it is free of secular solutions with linear growth, (ii) it produces energy-conserving schemes with appropriate time discretization, (iii) it can be easily extended to complex media (i.e. with frequency dispersion or anisotropy), (iv) it can be naturally hybridized with FDTD. In the remaining sections of Chapter 3, it is extended to inhomogeneous doubly-dispersive media [13]. The dispersion model used in the proposed scheme is very general and it can recover traditional models such as Debye, Lorentz or Drude media [1]. The implementation is based on
factorization of the mass matrix into simpler terms which produce an update scheme similar to that of FDTD with higher number of terms. Since the method is based on an element-based material profile, and this property is retained in the derivations, a favorable symmetric equation system is produced.

In chapter 3, a conformal perfectly-matched-layer (conformal-PML) implementation for the proposed method is presented [14]. Similar to doubly-dispersive materials, conformal PML can easily be incorporated into the proposed scheme and provide accurate simulation of open domain boundaries. Conformal-PML can eliminate the buffer regions that exists in the rectangular implementation of the problem and it can provide significant computational savings. Accuracy of the proposed method is demonstrated via numerical examples. A performance analysis of the conformal-PML with respect to algorithm constants is also presented in this chapter.

In chapter 4, a hybrid FDTD-FETD method is presented. In this method, fine detailed parts of the computational domain are modeled by finite-elements, whereas the remaining parts are modeled by finite-difference. This can produce significant computational savings by reducing the size of the matrix associated with the finite-element problem. Accuracy and efficiency of the method is studied via both 2D and 3D examples. In the latter, in order to perform geometrical transition from tetrahedral geometry of finite-elements, to the cubical geometry of finite-difference, pyramidal elements [15–17] are employed. In order to retain the favorable characteristics of the finite-element scheme based on differential forms, a compatible pyramidal element is used [17].
The focus of Chapter 5 is the full-electromagnetic particle-in-cell (PIC) method, which consists of a combination of first order Maxwell’s equations and particle kinematics [4, 5]. PIC simulations also suffer the same problems that exist in standard FDTD, such as high computational complexity and low geometrical flexibility. Moreover, problems are in multi-grid PIC implementations are much higher than that in pure electromagnetic problems due to the non-linear nature of the particle interactions. In order to alleviate the numerical artifacts, a subgridding by domain-overriding (SGDO) methodology [6] combined with Marder relaxation [18] is used to address this problem. Efficacy of the proposed method is demonstrated through numerical examples.
Finite-element time-domain methods have been successfully employed over the years for the simulation of transient Maxwell equations in complex geometries [2, 3, 19, 20]. In contrast to the finite-difference time-domain method [1], the finite element time-domain method requires the solution of sparse linear system at every time step; however, when used in conjunction with simplicial grids, the latter is free from stair-casing error. Traditionally, the finite element time-domain method is based on the solution of the second-order vector wave equation for the electric (or magnetic) field after the elimination of the magnetic (or electric) field [2]. This facilitates the expansion of the unknown field by a single type of basis functions. For the electric field, the basis functions of choice are typically edge elements. The choice of edge elements ensures conformity to a discrete version of the de Rham complex (exact sequence property) [21, 22]. This implies that discrete solutions that are not divergence-free necessarily correspond to static fields (gradient-like eigenmodes at zero frequency) which do not pollute the frequency spectrum. Edge elements can be viewed as the natural interpolants of 1-forms and hence provide the correct discrete representation for the electric field intensity, which in its most general mathematical incarnation is represented as a 1-form in a differential manifold [21–33].
In the frequency-domain second-order vector wave equation, the divergence-free nature of the (source-free) solutions is enforced in a frequency-dependent fashion (more precisely, quadratically with frequency). Hence, the divergence-free condition becomes progressively weak in the zero-frequency limit, leading to ill-conditioned matrices which negatively impacts accuracy and convergence [34]. This problem also plagues adaptive mesh refinement because the field approaches the static limit locally for elements in highly refined portions of the grid. In time-domain, a different but related kind of problem arises: the source-free second-order wave equation admits secular solutions of the form \( \vec{E} = (c_1 + c_2t)\nabla \phi \). These are spurious (nonphysical) modes in the null space of the curl operator and in the null space of the second-order time-derivative. These spurious modes require elimination using, for example, a tree-cotree decomposition (gauging) [35, 36], grad-div regularization terms, or a posteriori filtering approaches [37].

Alternatively, the finite element time-domain method can be based directly upon the first-order coupled Maxwell curl equations. In this case, both electric and magnetic fields are employed as unknowns and mixed finite-elements are used. A mixed finite element time-domain method employing the electric field intensity \( \vec{E} \) and magnetic field flux \( \vec{B} \) as simultaneous state variables have been considered in, e.g., [38–42] where edge elements (Whitney 1-forms) are used for \( \vec{E} \) and face elements (Whitney 2-forms) are used for \( \vec{B} \). This choice satisfies a discrete version of the de Rham diagram as well. Other desirable characteristics of this method are: (i) it is free of secular solutions with linear growth, (ii) it produces energy-conserving (symplectic) algorithms [43] under an appropriate choice for the time integration scheme, (iii) it provides a natural path for hybridization with the finite-difference time-domain
method since the latter can be formulated in terms of edge and face elements (now hexahedral) as well, and (iv) it is more easily extended to complex media (with frequency dispersion and/or anisotropy) because the constitutive equations are naturally decoupled from the spatial derivatives.

Although this mixed $E$-$B$ finite element time-domain method utilizes two fields as unknowns, its computer time and memory costs are comparable to those of the second-order vector wave equation formulation. This is because the former requires discretization of first-order time-derivatives while the latter requires second-derivatives. As a result, only one past time-step electric/magnetic field value is necessary during the time update of the mixed $E$-$B$ finite element time-domain method, as opposed to two past field values from using second-order time derivatives. In addition, in the mixed finite element time-domain method, the sparse linear system solution is required only for the electric field update, not for the magnetic field update. Consequently, the resulting linear system solution has the same number of unknowns as the in second-order wave equation formulation.

The use of finite element time-domain methods to simulate linear dispersive dielectrics has been considered before in [44–48]. These approaches were based on the second-order wave equation and included dispersion only in the permittivity. In this work, we take advantage of property (iv) above to construct a mixed $E$-$B$ finite element time-domain method for inhomogeneous and doubly-dispersive media where both the permittivity and permeability are functions of frequency [13]. This type of behavior is found, for example, in many metamaterials [49,50]. The dispersion models that we consider here are very general and recover Debye, Lorentz, and Drude models

\footnote{These numbers refer to a first-order time discretization in dispersionless media only, but a similar comparison can be made for high-order time discretizations and for dispersive media.}
as special cases. The algorithm also incorporates the perfectly matched layers [1] in a natural way.

2.1 Homogeneous media

2.1.1 Three-dimensional case

We expand the electric field intensity $\bar{E}$ in terms of Whitney edge elements $\bar{W}_i^1$, $i = 1, \ldots, N_e$, and the magnetic field flux density $\bar{B}$ in terms of Whitney face elements $\bar{W}_i^2$, $i = 1, \ldots, N_f$, as [39]

$$
\bar{E} = \sum_{i=1}^{N_e} e_i \bar{W}_i^1 \quad \bar{B} = \sum_{i=1}^{N_f} b_i \bar{W}_i^2 \quad (2.1)
$$

where $e_i$ and $b_i$ are the unknown of the problem, and $N_e$ and $N_f$ are number of interior (or free) edges and faces, respectively. The expansion above refers to the three-dimensional case where, $E$ is a 1-form expanded in terms of Whitney 1-forms $\bar{W}_i^1$ (edge elements) and $B$ is a 2-form expanded in terms of Whitney 2-forms $\bar{W}_i^2$ (face elements) as expressed in (2.1).

By denoting arrays of unknowns (column vectors) as $\mathbb{E} = [e_1, e_2, \ldots, e_{N_e}]^T$ and $\mathbb{B} = [b_1, b_2, \ldots, b_{N_f}]^T$, the semi-discrete Maxwell equations in a source-free region can be written as

$$
\mathbb{D} = [\star_\epsilon] \mathbb{E} \quad (2.2)
$$
$$
\mathbb{H} = [\star_{\mu-1}] \mathbb{B} \quad (2.3)
$$
$$
-j\omega \mathbb{D} = [\mathcal{D}_{\text{curl}}^*] \mathbb{H} - \mathbb{J}_s \quad (2.4)
$$
$$
-j\omega \mathbb{B} = -[\mathcal{D}_{\text{curl}}] \mathbb{E} - \mathbb{M}_s \quad (2.5)
$$

where $[\mathcal{D}_{\text{curl}}]$ and $[\mathcal{D}_{\text{curl}}^*]$ are (metric-free) sparse incidence matrices on the primal (finite element mesh) and dual grid, respectively, whose elements assume only $\{-1, 0, 1\}$
values [24, 33]. The identity \([D_{\text{curl}}^*] = [D_{\text{curl}}]^T\) holds in general, up to boundary terms. The column vectors \(\mathbb{D} = [d_1, d_2, \ldots, d_{N_e}]^T\) and \(\mathbb{H} = [h_1, h_2, \ldots, h_{N_f}]^T\) represent the electric field flux density and the magnetic field intensity, respectively. The \(\mathbb{D}\) and \(\mathbb{H}\) arrays are not associated with the finite element mesh directly, but with dual mesh instead [33]. If we denote \(i\) and \(j\) as row and column indices respectively, the discrete Hodge matrices \([\star_e]\) (size \(N_e\) by \(N_e\)) and \([\star_{\mu^{-1}}]\) (size \(N_f\) by \(N_f\)) in (2.3), are given by the following integrals [39]

\[
[\star_e]_{ij} = \int_{\Omega} \bar{W}_i^1 \cdot \bar{\epsilon}(\bar{r}) \cdot \bar{W}_j^1 \, d\Omega \quad (2.6)
\]

\[
[\star_{\mu^{-1}}]_{ij} = \int_{\Omega} \bar{W}_i^2 \cdot \bar{\mu}^{-1}(\bar{r}) \cdot \bar{W}_j^2 \, d\Omega \quad (2.7)
\]

where \(\Omega\) is the computation domain, and \(\bar{\epsilon}(\bar{r})\) and \(\bar{\mu}(\bar{r})\) are permittivity and permeability tensors at location \(\bar{r}\), respectively. The integrals in (2.6) and (2.7) are volume integrals in three dimensions and area integrals in two dimensions. The semi-discrete Maxwell equations can be written by making appropriate substitutions and taking the inverse Fourier transform of (2.4)-(2.5) as [78], [33]

\[
[\star_e] \frac{\partial}{\partial t} \mathbb{E} = [D_{\text{curl}}^*][\star_{\mu^{-1}}]\mathbb{B} - \mathbb{J}_s \quad (2.8)
\]

\[
\frac{\partial}{\partial t} \mathbb{B} = -[D_{\text{curl}}]\mathbb{E} - \mathbb{M}_s \quad (2.9)
\]

In non-dispersive media and using a leap-frog time-discretization, the finite element time-domain update equations are given by [39].

\[
[\star_e] \mathbb{E}^n = [\star_e] \mathbb{E}^{n-1} + \Delta t[D_{\text{curl}}^*][\star_{\mu^{-1}}]\mathbb{B}^{n-\frac{1}{2}} - \Delta t\mathbb{J}_s^{n-\frac{1}{2}} \quad (2.10)
\]

\[
\mathbb{B}^{n+\frac{1}{2}} = \mathbb{B}^{n-\frac{1}{2}} - \Delta t[D_{\text{curl}}]\mathbb{E}^n - \Delta t\mathbb{M}_s^n \quad (2.11)
\]
The Hodge (mass) matrix \([\star \epsilon]\) is sparse but not diagonal, and the solution of the associated linear system is the most computationally intensive part of the update.

2.1.2 Two-dimensional TE\(_z\) and TM\(_z\) cases

In the two-dimensional TE\(_z\) case considered in the numerical examples that follow, \(E\) is still a 1-form and \(B\) is still a 2-form, so all the above formulas still apply. Note, however, that in two-dimensions, the Whitney form \(\bar{W}_i^2\) becomes a \(z\)-directed function which is uniform over each face (two-dimensional volume form).

On the other hand, in the two-dimensional TM\(_z\) case (not considered here), \(E\) is a 0-form and hence should be expanded in terms of Whitney 0-forms (nodal elements), while \(B\) is a 1-form and hence should be expanded in terms of Whitney 1-forms (edge elements).

A complete classification table with the degrees of the differential forms representing each field for different dimensions and polarizations is presented in [32]. Moreover, a discussion on the appropriate expansions (based on such classification) for the various dimensions/polarizations is provided in [40].

2.2 Inhomogeneous and doubly-dispersive media

2.2.1 Formulation

In inhomogeneous media, the material tensors are assumed uniform within each face, i.e., \(\bar{\epsilon}(\bar{r}) \rightarrow \bar{\epsilon}(k)\) and \(\bar{\mu}(\bar{r}) \rightarrow \bar{\mu}(k)\), where \(k\) is the face index. Material tensors could alternatively have been associated with edges; however, since an implementation of (2.6) requires knowledge of the material parameters pointwise, an interpolation
of the material parameters would have been necessary. Moreover, an edge-based definition for the material tensors in inhomogeneous media would lead to non-symmetric Hodge matrices.

We consider a two-dimensional TE$_z$ problem in Cartesian coordinates with inhomogeneous and dispersive diagonal material tensors given as

\[
\tilde{\epsilon}(k; \omega) = \hat{x}\hat{x} \epsilon_x(k; \omega) + \hat{y}\hat{y} \epsilon_y(k; \omega)
\]  
\[
\tilde{\mu}(k; \omega) = \hat{z}\hat{z} \mu_z(k; \omega)
\]

with

\[
\epsilon_x(k; \omega) = \frac{\sum_{p=0}^{N_p} g_x^p(k)(j\omega)^p}{\sum_{p=0}^{N_p} r_x^p(k)(j\omega)^p}
\]

and similarly for $\epsilon_y(k; \omega)$ and $\mu_z(k; \omega)$. Even though the above tensors are specific for two dimensions, a three-dimensional formulation can be derived following similar steps as below.

### 2.2.2 Electric field constitutive equation update

In this section, we decompose $\mathbb{D}$ in (2.3) in a form suitable for time-discretization. If we denote $\Omega_k$ as the area of the $k$-th face, (2.6) can be rewritten as a sum of face contributions as

\[
[*]_{ij} = \sum_{k=1}^{N_f} \int_{\Omega_k} \tilde{W}_i^1 \cdot \tilde{\epsilon}(k) \cdot \tilde{W}_j^1 d\Omega
\]
Substituting (2.12) into (2.15) and separating terms for different axis components, we get

\[
\begin{align*}
[\star \epsilon]_{ij} &= \sum_{k=1}^{N_f} \int_{\Omega_k} \epsilon_x(k) \left( \hat{x} \cdot \hat{W}_i^1 \right) \left( \hat{x} \cdot \hat{W}_j^1 \right) d\Omega \\
&\quad + \sum_{k=1}^{N_f} \int_{\Omega_k} \epsilon_y(k) \left( \hat{y} \cdot \hat{W}_i^1 \right) \left( \hat{y} \cdot \hat{W}_j^1 \right) d\Omega 
\end{align*}
\]

(2.16)

where we have dropped the frequency dependence for simplicity. Since material parameters are assumed uniform inside each element, (2.16) can be further simplified to

\[
[\star \epsilon] = \sum_{k=1}^{N_f} \epsilon_x(k) [L_x(k)] + \sum_{k=1}^{N_f} \epsilon_y(k) [L_y(k)]
\]

(2.17)

with

\[
[L_x(k)]_{ij} = \int_{\Omega_k} \left( \hat{x} \cdot \hat{W}_i^1 \right) \left( \hat{x} \cdot \hat{W}_j^1 \right) d\Omega
\]

(2.18)

and similarly for \([L_y(k)]_{ij}\). Substituting (2.17) into (2.3), \(D\) is written as

\[
D = \sum_{k=1}^{N_f} \epsilon_x(k) [L_x(k)]E + \sum_{k=1}^{N_f} \epsilon_y(k) [L_y(k)]E
\]

(2.19)

Although the summation above includes all \(k\) faces, the inner-product integrals \([L_x(k)]_{ij}\) and \([L_y(k)]_{ij}\) are non-zero for two faces only, viz., the two faces that touch edge \(j\), denoted here as \(k_{\uparrow j}\) and \(k_{\downarrow j}\) respectively (see Fig. 2.1). Consequently, the summation over faces in (2.19) reduces to a summation of two terms with faces indices \(k_{\uparrow j}\) and \(k_{\downarrow j}\). As a result, each element \(d_j\) of the array \(D\) can be written as

\[
d_j = \sum_{i=1}^{N_e} \epsilon_x(k_{\uparrow j}) [L_x(k_{\uparrow j})]_{ij} e_i + \sum_{i=1}^{N_e} \epsilon_x(k_{\downarrow j}) [L_x(k_{\downarrow j})]_{ij} e_i \\
+ \sum_{i=1}^{N_e} \epsilon_y(k_{\uparrow j}) [L_y(k_{\uparrow j})]_{ij} e_i + \sum_{i=1}^{N_e} \epsilon_y(k_{\downarrow j}) [L_y(k_{\downarrow j})]_{ij} e_i
\]

(2.20)
We can further write

\[ d_j = d_{x\uparrow j} + d_{x\downarrow j} + d_{y\uparrow j} + d_{y\downarrow j} \]  

(2.21)

where

\[ d_{x\uparrow j} = \epsilon_x(k_{\uparrow j})e_{x\uparrow j} \]  

(2.22)

and

\[ e_{x\uparrow j} = \sum_{i=1}^{N_e} \mathcal{L}_x(k_{\uparrow j})_{ij} e_i \]  

(2.23)

and similarly for \( d_{x\downarrow j}, d_{y\uparrow j}, d_{y\downarrow j}, e_{x\downarrow j}, e_{y\uparrow j}, \) and \( e_{y\downarrow j}, \) with \( j = 1, \ldots, N_e. \)

We note that the form of (2.20) resembles that of the finite-difference time-domain algorithm in dispersive and inhomogeneous media, where the field variables multiply a dispersion function that depends on each grid point. However, four different functions per edge, viz., \( \epsilon_x(k_{\uparrow j}), \epsilon_x(k_{\downarrow j}), \epsilon_y(k_{\uparrow j}), \epsilon_y(k_{\downarrow j}) \) are used here, as opposed to a single one in the finite-difference time-domain algorithm. This comes from the fact that each edge contacts two faces with possibly independent dispersion characteristics and each of
these two faces may have independent dispersion characteristics along each of the two
axis $x$ and $y$ in two dimensions.

In the time-domain, the dispersion relation (2.22) becomes an ordinary differential
equation and a time discretization is performed to obtain update equations. For
example, if we denote $d_{x|1}^{(p)}$ and $e_{x|1}^{(p)}$ as the $p$-th order time-derivatives of $d_{x|1}$ and $e_{x|1}$,
respectively, and substitute (2.14) into the dispersion relation (2.22), we obtain

$$
\sum_{p=0}^{N_p} r_x^{(p)}(k_{|1}) d_{x|1}^{(p)} = \sum_{p=0}^{N_p} q_x^{(p)}(k_{|1}) e_{x|1}^{(p)}
$$

(2.24)

We discretize the above at discrete time-steps $t = n\Delta t$, and apply the following
finite-difference approximation recursively

$$
e_{x|1}^{(p)}|^{n+1} \approx -e_{x|1}^{(p)}|^{n} + \frac{2}{\Delta t} \left(e_{x|1}^{(p-1)}|^{n+1} - e_{x|1}^{(p-1)}|^{n}\right)
$$

(2.25)

and similarly for $d_{x|1}^{(p)}|^{n+1}$. The update equation for $d_{x|1}^{(p)}|^{n+1}$ can then be written as

$$
d_{x|1}^{(p)}|^{n+1} = w_x(k_{|1}) e_{x|1}^{(p)}|^{n+1} + g_{x|1}^{(p)}|^{n}
$$

(2.26)

$$
g_{x|1}^{(p)}|^{n} = \left(\sum_{p=0}^{N_p} u_x^{(p)}(k_{|1}) d_{x|1}^{(p)}|^{n}\right)
- \left(\sum_{p=0}^{N_p} v_x^{(p)}(k_{|1}) e_{x|1}^{(p)}|^{n}\right)
$$

(2.27)

where $w_x(k_{|1})$, $u_x^{(p)}(k_{|1})$, and $v_x^{(p)}(k_{|1})$ are constants that depend on material parameters $q_x^{(p)}(k_{|1})$ and $r_x^{(p)}(k_{|1})$. Expressions for these constants are given in the Appendix
A for a dispersive model with $N_p = 4$. The auxiliary variable $g_{x|1}^{(p)}|^{n}$ is defined for
convenience and depends only on values of $e_{x|1}$ and $d_{x|1}$ from previous time-steps.

Update equations for $d_{x|1}$, $d_{y|1}$, $d_{y|1}$ are obtained following similar steps.

By denoting $D_{x|1} = [d_{x|1}, d_{x|2}, \ldots, d_{x|N_x}]^T$ and similarly for $G_{x|1}$, we can combine
(2.23) and (2.26) in matrix form as

$$
D_{x|1}^{n+1} = W_{x|1} D_{x|1}^{n} + G_{x|1}^{n}
$$

(2.28)
where \([\mathcal{L}_x]_{ij} = [\mathcal{L}_x(k_{ij})]_{ij}\) and \([\mathcal{W}_x] = \text{diag}\{w_x(k \uparrow 1), w_x(k \uparrow 2), \ldots, w_x(k \uparrow N_e)\}\), and similarly for \(\mathbb{D}^{n+1}_x, \mathbb{D}^{n+1}_y,\) and \(\mathbb{D}^{n+1}_z\). From (2.21), we have

\[
\mathbb{D} = \mathbb{D}_x + \mathbb{D}_y + \mathbb{D}_z
\]  

(2.29)

and similarly for \(\mathbb{G}\). Using (2.28) and (2.29), we finally arrive at

\[
[\mathcal{A}]\mathbb{E}^{n+1} = \mathbb{D}^{n+1} - \mathbb{G}^n
\]  

(2.30)

where

\[
[\mathcal{A}] = [\mathcal{W}_x][\mathcal{L}_x] + [\mathcal{W}_x][\mathcal{L}_x] \\
+ [\mathcal{W}_y][\mathcal{L}_y] + [\mathcal{W}_y][\mathcal{L}_y]
\]  

(2.31)

The above constitutes the update equation for \(\mathbb{E}\) given \(\mathbb{D}\). As mentioned before, the solution of the sparse linear system associated with \([\mathcal{A}]\) usually constitutes the most computationally intensive part of the update.

### 2.2.3 Magnetic field constitutive equation update

Following the same methodology of part (a), the Hodge matrix \([\ast_{\mu-1}]\) can be written as

\[
[\ast_{\mu-1}] = \sum_{k=1}^{N_f} \mu_{\varepsilon}^{-1}(k)[\mathcal{L}_z(k)]
\]  

(2.32)

with

\[
[\mathcal{L}_z(k)]_{ij} = \int_{\Omega} (\hat{z} \cdot \hat{\nu}_i^2) (\hat{z} \cdot \hat{\nu}_j^2) \, d\Omega
\]  

(2.33)

\[
= \begin{cases} 
\Omega_k^{-1}, & \text{if faces } (i, j) = (k, k) \\
0, & \text{otherwise}
\end{cases}
\]  

(2.34)
Substituting (2.34) and (2.32) into (2.3), we obtain the following equation for $h_k$

$$h_k = \Omega_k^{-1} \mu_z^{-1}(k) h_k$$

(2.35)

for $k = 1, \ldots, N_f$.

The update for $\mathbb{H}$ from (2.35) is derived in a similar fashion as the update for $\mathbb{E}$. The main difference is that while the support of each edge element $\bar{W}_1^i$ consists of two faces, the support of each face (cell) element $\bar{W}_2^i$ consists of only face $i$, and as such, there is no need for the field splitting such as done in (2.21). Furthermore, matrix $[\mu^{-1}]$ is diagonal in the two-dimensional TE case. From (2.35) and after application of similar steps to those in (2.24)–(2.30), one arrives at the following equation

$$[\mathcal{A}_\mu]^{\mathbb{H}}_{n+\frac{1}{2}} = \mathbb{B}^{n+\frac{1}{2}} - \mathbb{G}^{n+\frac{1}{2}}$$

(2.36)

where $[\mathcal{A}_\mu]$ and $\mathbb{G}^n$ are analogous to $[\mathcal{A}]$ and $\mathbb{G}^n$ respectively, now for the permeability. The matrix $[\mathcal{A}_\mu]$ is a (diagonal) matrix given by the product of two diagonal matrices

$$[\mathcal{A}_\mu] = [W_z][L_z]$$

(2.37)

where $[L_z]_{ij} = [L_z(k=j)]_{ij}$. Because $[\mathcal{A}_\mu]$ is diagonal, its inversion is trivial (explicit $\mathbb{H}$ update).

### 2.2.4 Curl equations and complete update

The update equations for $\mathbb{D}$ and $\mathbb{B}$ are both explicit and follow directly from Maxwell curl equations (2.5) as

$$\mathbb{D}^{n+1} = \mathbb{D}^n + \Delta t[\mathcal{D}_{\text{curl}}]\mathbb{H}^{n+\frac{1}{2}} - \Delta t\mathbb{H}_s^{n+\frac{1}{2}}$$

(2.38)

$$\mathbb{B}^{n+\frac{1}{2}} = \mathbb{B}^{n-\frac{1}{2}} - \Delta t[\mathcal{D}_{\text{curl}}]\mathbb{E}^n - \Delta t\mathbb{M}_s^n$$

(2.39)

A complete time step update consists of application of (2.39), (2.36), (2.38), and (2.30), in this sequence.
2.3 Perfectly Matched Layers

A rectangular (Cartesian) perfectly matched layer [1] implementation is used to truncate the computational domain and simulate an open-domain problem. The implementation described here is based on the first-order Maxwell equations and it is a particular case of the double-dispersive anisotropic material modeling discussed above. The reader is referred to [51] for an implementation of the rectangular perfectly matched layer in time-domain finite-element simulations based on the second order wave equation.

Given an anisotropic and dispersive interior media with constitutive tensors $\bar{\epsilon}$ and $\bar{\mu}$, the associated tensors $\bar{\epsilon}_{\text{pml}}$ and $\bar{\mu}_{\text{pml}}$ to achieve reflectionless absorption are given by [52]

$$
\bar{\epsilon}_{\text{pml}} = \left( \text{det } \bar{S} \right)^{-1} \bar{S} \cdot \bar{\epsilon} \cdot \bar{S}, \quad (2.40)
$$

$$
\bar{\mu}_{\text{pml}} = \left( \text{det } \bar{S} \right)^{-1} \bar{S} \cdot \bar{\mu} \cdot \bar{S}, \quad (2.41)
$$

with

$$
\bar{S} = \hat{x}\hat{x} \frac{1}{s_x} + \hat{y}\hat{y} \frac{1}{s_y} + \hat{z}\hat{z} \frac{1}{s_z}. \quad (2.42)
$$

where $s_x, s_y,$ and $s_z$ are complex stretching variables [85]. For diagonal tensors $\bar{\epsilon}, \bar{\mu}$, the above simplifies to

$$
\bar{\epsilon}_{\text{pml}}(k; \omega) = \bar{\epsilon}(k; \omega) \bar{\Lambda}(k; \omega), \quad (2.43)
$$

$$
\bar{\mu}_{\text{pml}}(k; \omega) = \bar{\mu}(k; \omega) \bar{\Lambda}(k; \omega), \quad (2.44)
$$

with $\bar{\Lambda} = \left( \text{det } \bar{S} \right)^{-1} \bar{S} \cdot \bar{S}$, For the two-dimensional (TE$_z$) cases considered in the examples that follow, and using conventional stretching variables of the form $s_x = \ldots$
$1 + \sigma_x/(j\omega\epsilon_0)$, and similarly for $s_y$, the PML tensor elements reduce to

\[
\begin{align*}
\epsilon_{pml}^x(k;\omega) &= \epsilon_x(k;\omega) \left(\frac{j\omega\epsilon_0 + s_y}{j\omega\epsilon_0 + \sigma_x}\right) \\
\epsilon_{pml}^y(k;\omega) &= \epsilon_y(k;\omega) \left(\frac{j\omega\epsilon_0 + \sigma_x}{j\omega\epsilon_0 + s_y}\right) \\
\mu_{pml}^z(k,\omega) &= \mu_z(k;\omega) \left[\frac{(j\omega\epsilon_0)^2}{(j\omega\epsilon_0 + \sigma_x)(j\omega\epsilon_0 + s_y)}\right]
\end{align*}
\]

(2.45) (2.46) (2.47)

If the background material parameters in (2.45)–(2.47) $\epsilon_x(k;\omega), \epsilon_y(k;\omega), \mu_z(k;\omega)$ are modeled by second order polynomials in $\omega$, the tensors $\bar{\epsilon}_{pml}$ and $\bar{\mu}_{pml}$ can be realized by a fourth order polynomial, $N_p = 4$.

### 2.4 Numerical results

We consider a two-dimensional TE$_z$ problem with a broadband, soft magnetic point source. The time-domain excitation given by $f(t) = -0.488 \sin(2\pi v_c/\lambda_0) + 0.290 \sin(4\pi v_c/\lambda_0) - 0.031 \sin(6\pi v_c/\lambda_0)$ for $0 < t < \lambda_0/v_c$ and $f(t) = 0$ otherwise (Blackman-Harris pulse derivative). This excitation is used in all test cases unless stated otherwise. Here, $\lambda_0$ is the free-space wavelength associated with the central frequency, and $v_c$ is the speed of light. The time step is chosen according to length of the shortest edge of the mesh, $l_{min}$, and given by $\Delta t = c_N l_{min}/v_c$. The Courant number is chosen as $c_N = 0.2$. In all simulations below, a mesh generation algorithm with a maximum area constraint $\Omega_k < \sqrt{3}l_e^2/4$ for all elements $k$ is used, where $l_e$ is the mesh resolution in terms of an edge length. A sparse incomplete Cholesky factorization with a drop tolerance value $10^{-10}$ is used for solving (2.30).

#### 2.4.1 Validation: Cylindrical scatterer

In order to verify the accuracy of the scheme, we simulate the fields due to a point source in the vicinity of a frequency-dispersive circular cylinder, as depicted
in Fig. 2.2. A computational domain with size $0.56 \times 0.56\text{m}^2$ is used with average mesh resolution $l_e = 0.04\text{ m}$. The (free-space) central wavelength is $\lambda_0 = 2\text{ m}$ and the dispersive cylinder has radius $r = 0.2\text{ m}$. The field is sampled at the center of the cylinder (where it is more sensitive to the dispersive properties) and the point source is located at $0.4\text{ m}$ away from the receiver. Perfectly matched layers are used for mesh termination (as detailed above). Two scenarios are considered: (i) cylinder filled with a dielectric dispersive material and (ii) cylinder filled with a doubly-dispersive material. The two-pole Debye model described below is used for the dispersive permittivity and permeability. A static conductivity term is also included as an additional parameter to this model.

$$\epsilon_x(\omega) = \epsilon_y(\omega) = \epsilon_0\epsilon_\infty + \frac{\sigma}{j\omega} + \epsilon_0\sum_{i=1}^{2} \frac{A^\epsilon_i}{1 + j\omega\tau^\epsilon_i} \quad (2.48)$$

San Antonio clay loam parameters [53] are used for the dispersive permittivity model, and given by $\epsilon_\infty = 3.64$, $A^\epsilon_1 = 1.67$, $A^\epsilon_2 = 0.48$, $\tau^\epsilon_1 = 1.70\text{ nsec}$, $\tau^\epsilon_2 = 0.12\text{ nsec}$, $\sigma = 1.4\text{ mS/m}$ and $\mu = \mu_0$. For a doubly-dispersive cylinder, we consider the same permittivity together with a two-pole Debye permeability with $\mu_\infty = 1.55$, $A^\mu_1 = 1.67$, $A^\mu_2 = 0.48$, $\tau^\mu_1 = 2.80\text{ nsec}$ and $\tau^\mu_2 = 0.18\text{ nsec}$.

Finite element time-domain results are compared against finite-difference time-domain results and an analytical solution. The analytical solution is obtained from the Green’s function for this problem, which can be expressed in terms of a Hankel-Bessel series over the azimuth index [54, pp. 574-667], with the first 50 terms included. The time-domain source excitation is first converted to frequency-domain by a Fourier transformation. Zero padding with a length that is 10 times the total number of time steps is used in this operation to ensure good enough frequency resolution. At each frequency, the source spectrum is multiplied by the analytical solution.
Figure 2.2: Finite-element mesh for the dispersive cylindrical scatterer. The source location is indicated by the + and the probe location by the ×.
that frequency. The result is inverse Fourier transformed to yield the time-domain response. The total number of cells of the uniform finite-difference time domain grid is equal to the number of faces in the finite element mesh. Figs. 2.3(a) and 2.4(a) show the calculated magnetic field values as a function of time at the probe position. Figs. 2.3(b) and 2.4(b) show the relative errors against the analytical result, indicating that the proposed method can accurately simulate materials with dispersive and doubly-dispersive characteristics. The finite-difference time-domain method produces a higher residual error for this geometry and mesh resolution because mainly of staircasing approximations.

### 2.4.2 Perfectly matched layer performance

In order to test the perfectly matched layer performance, a domain with size $\lambda_0 \times \lambda_0$, and mesh resolution $l_e = \lambda_0/60$, is used. The domain is extruded by $N_{pml} = 4, 8, 16, \text{ and } 24$ perfectly matched layer cells, where a polynomial profile with exponent $n = 2.5$ is used for the conductivity [1]. A planarly layered mesh with rectangular tiles made of two triangular cells each is used in the perfectly matched layer. The edge length of each tile is chosen approximately equal to $0.7l_e$. The reference finite element time-domain result for subtraction to calculate the perfectly matched layer reflection coefficient is obtained with a larger mesh constructed by extruding the same mesh by a large number of free-space layers. The same exact rectangular tile geometry is used in the extrusion region to avoid any differences in the numerical dispersion effects and isolate the residual reflections from the perfectly matched layer. For reflection coefficient normalization purposes, a third mesh is constructed by terminating the original mesh by perfect electrical conducting walls. In the numerical tests, the source
Figure 2.3: Calculated field and normalized residual error produced by the mixed finite element time-domain (FETD) and finite-difference time-domain (FDTD) methods for the San Antonio clay loam cylinder model. The peak residual error of FETD is about −50 dB.
Figure 2.4: Calculated field and normalized residual error produced by the mixed finite element time-domain (FETD) and finite-difference time-domain (FDTD) methods for the doubly-dispersive cylinder model. The peak residual error of FETD method is about $-54$ dB.
is placed at the center of the domain at $x_{src} = \lambda_0/2$ and $y_{src} = \lambda_c/2$. The receiver
is placed at $x_{src} = 2\lambda_0/3$ and $y_{src} = \lambda_0/2$. We denote $h^{pml|n}_{krec}$, $h^{pec|n}_{krec}$ and $h^{ref|n}_{krec}$ as
the magnetic field at grid cell (face) $krec$ at time-step $n$ in the perfectly matched
layer case, the cavity case, and reference case, respectively. The residual reflection
coefficient from the perfectly matched layer is calculated by

$$R_{pml}(n) = 20 \log_{10} \left( \frac{\max_n |h^{pml|n}_{krec} - h^{ref|n}_{krec}|}{\max_n |h^{pec|n}_{krec} - h^{ref|n}_{krec}|} \right)$$

(2.49)

The reflection coefficient for different perfectly matched layer thickness in terms of

![Figure 2.5: Perfectly matched layer (PML) numerical reflection coefficient for various
number of layer cells. A reflection level no larger than $-55$ dB is obtained for 8 layers
for the source excitation considered.](image)

number of cells is plotted in Fig. 2.5. A reflection level no larger than about $-55$ dB
is obtained for 8 cells. Lower reflection levels are obtained by further increasing the
perfectly matched layer thickness.
2.4.3 Zero-index lens

Zero-index metamaterials are doubly-dispersive media that exhibit zero permittivity and zero permeability at a specified frequency. Interestingly, the electromagnetic fields inside such materials (at the critical frequency) have a spatial distribution akin to that of a static field (i.e., infinitely long wavelength) while remaining dynamic (oscillatory) in time [49]. Here, we consider a lens object made of a homogeneous zero-index metamaterial in free space as shown in Fig. 2.6. The zero-index material is realized by the isotropic Drude model below [49]

\[
\epsilon_x(\omega) = \epsilon_y(\omega) = \epsilon_0 \left[ 1 - \frac{\omega_p^2}{\omega(\omega - j\Gamma_e)} \right] \tag{2.50}
\]

\[
\mu_z(\omega) = \mu_0 \left[ 1 - \frac{\omega_p^2}{\omega(\omega - j\Gamma_e)} \right] \tag{2.51}
\]

The zero-index frequency is given by \( \omega_p = 6.2832 \times 10^{10} \) with \( \Gamma_e = 1 \times 10^{-5} \omega_p \). The lens has a double-concave semi-circular geometry with 12 cm width and 7.4 cm height. The radii of curvature of the semi-circular regions are 12.2 cm and 21.8 cm. A 18 cm \( \times \) 23.5 cm domain is used for the finite element time-domain simulation, with average mesh resolution \( l_e = 0.3 \) cm. A ramped-sine source [55] is used with half-period ramp length and sine frequency \( \omega_p \). The source is located at the center of the top circular disk associated with the lens geometry.

Fig. 2.6 shows a snapshot of magnetic field values taken at \( t = 8.8151 \times 10^{-10} \) s, where it is seen that the cylindrical wave originated from the source above the lens is focused below the lens (wavefront reshaping property). The uniform field values inside the lens indicate the static-like spatial distribution of the field inside the zero-index lens.
Figure 2.6: Snapshot of the magnetic field at $t = 8.8151 \times 10^{-10}$ s for the zero-index lens problem. The lens is made of a homogeneous doubly-dispersive material. The field originating from a point source is refocused below the lens, demonstrating a wavefront reshaping property of this lens.
2.4.4 Metamaterial blueprints for reflectionless waveguide bends

A fundamental property of Maxwell’s equations is that a continuous transformation on the metric of space can be made equivalent to a change in the material tensors. This “metric invariance” property of Maxwell’s equations has long been known [28,31,56–59], and it is best expressed using exterior differential forms [31,60]. Motivated by recent advances in metamaterials fabrication, this property was recently explored for cloaking [61–63] and masking [64,65] of scatterers, and waveguide miniaturization [66].

The metamaterial blueprints are obtained using a bijective coordinate transformation that allows for all waveguide modes to be guided without any reflection or cross-coupling through the bend (perfect matching). Simulations based on E-B Mixed FETD are carried out in this section to demonstrate the proposed functionality and examine its sensitivity to small perturbations [67].

The proposed functionality is demonstrated in a two-dimensional TM$_z$ problem consisting of a parallel-plate waveguide bend with the geometry depicted in Fig. 2.7.

The waveguide is filled with air in the straight sections and with the meta-material blueprint given in [67]. We assume waveguide thickness $w = \lambda_s/4 = 1.5$ cm, bending angle of 135° and radius of curvature $r = 0.8488$ cm. The bending section starts at $x_t = 10$ cm. The source is a $z$-directed magnetic dipole excited by a Blackman-Harris pulse derivative $f(t) = -0.488 \sin(2t\pi v_c/\lambda) + 0.290 \sin(4t\pi v_c/\lambda) - 0.031 \sin(6\pi v_c/\lambda)$ for $0 < t < \lambda/v_c$ and $f(t) = 0$ otherwise, where $v_c$ is the speed of light in vacuum. Two particular excitations are considered. For the first excitation, the central wavelength is $\lambda_s = 6$ cm (5 GHz), and source and probe are placed at mid-height in the waveguide.
along the $y$ direction, and at $x_s = 0.2$ cm and $x_p = 9.5$ cm along $x$, respectively. In this case, only the TM$_0$ mode (TEM-like) propagates in the parallel-plate waveguide. For the second excitation, the central wavelength is chosen as $\lambda_s = 3$ cm (10 GHz), and source and probe are placed at $y_s = y_p = w/3$, so that both TM$_0$ and TM$_1$ propagating modes are produced.

The total and reflected field values at the probe location are plotted in Fig. 2.8(a) for (1) bent waveguide with no metamaterial, (2) bent waveguide with metamaterial, and (3) straight waveguide (as a reference). Two further simulations with slightly perturbed tensors are performed to examine the sensitivity of the response. This is done by employing coarser meshes where the tensors are modeled by different numbers of piecewise constant material blocks, $N_e = 4837$ and $N_e = 1597$ (note the original finite-element mesh has $N_e = 8050$, where each element effectively acts as a material block as well).
Figure 2.8: Total (main plot) and reflected (inset in dB scale) fields in the bend waveguide. The results without coarsening (about 8000 elements) do not appear in the inset plots because the reflection levels are well below $-70$ dB.
Fig. 2.8(a) shows that the bent section with metamaterial loading does not produce any reflections above $-70$ dB under TM$_0$ excitation, and that both coarsely distributed cases are also effective in supressing reflection. Fig. 2.8(b) shows the performance under combined TM$_0$, TM$_1$ excitation. Again, the metamaterial is highly effective in supressing reflections, but the results are more sensitive to the coarsening of the distribution, especially for frequencies closer to the cut-off (lower phase velocities), which contribute to the late time response.

The discussion is this section has concerned with the derivation of the metamaterial tensors at the “blueprint level” [68] only. Aspects of the physical realizability have not been discussed, but it is important to point out here some fundamental limitations. As shown in [67], the magnitude of the permittivity eigenvalues varies between $0.1\epsilon_0$ and $8.5\epsilon_0$ and a similar demand is posed on the permeability tensor. This implies a (intrinsic) phase velocity above $v_c$, which is admissible only if the material tensors are frequency dispersive, and hence lossy as implied by Kramers-Kronig relations [68]. Since the material blueprints considered here are frequency independent, the above implies that any physical realization based on them is necessarily narrowband and has a performance limited by losses. This limitation is also present in cloaking and masking metamaterial blueprints [61, 64, 65, 69].

2.5 Stability in inhomogeneous media

In this section a proof for stability of the FETD method will be presented. It is based on similar proofs in [11, 70] for FDTD. In contrast to proofs based on von Neummann analysis, the following proof is valid for practical scenarios including inhomogeneous materials and bounded domains [71]. The proof is presented in three
In the first part, a convenient representation for the system matrix associated with the discrete update equations is obtained. In the second part, a similar representation for the semi-discrete update equations is obtained. Finally in the final part, result of the semi-discrete system is used as an additional constraint in the discrete system to obtain the stability criterion.

### 2.5.1 System matrix for discrete update equations

In order to obtain a convenient representation for the system matrix associated with the discrete update equations, future field values are expressed in terms of past field values. In particular (2.10) is substituted in (2.11) and the resulting equations read as

\[
E^n = E^{n-1} + \Delta t [\star \epsilon]^{-1} [D_{curl}]^*[\star \mu^{-1}] B^{n-\frac{1}{2}}
\]

\[
B^{n+\frac{1}{2}} = B^{n-\frac{1}{2}} - \Delta t [D_{curl}] E^{n-1} - \Delta t^2 [\star \epsilon]^{-1} [D_{curl}]^*[\star \mu^{-1}] B^{n-\frac{1}{2}}
\]

where source terms are omitted for simplicity. Equns. (2.52)-(2.53) can be rewritten in matrix form by augmenting \( E \) and \( B \) vectors as

\[
\begin{bmatrix}
    E^n \\
    B^{n+\frac{1}{2}}
\end{bmatrix} =
\begin{bmatrix}
    I & \Delta t [\star \epsilon]^{-1} [D_{curl}]^*[\star \mu^{-1}] \\
    -\Delta t [D_{curl}] & I - \Delta t^2 [\star \epsilon]^{-1} [D_{curl}]^*[\star \mu^{-1}]
\end{bmatrix}
\begin{bmatrix}
    E^{n-1} \\
    B^{n-\frac{1}{2}}
\end{bmatrix}
\]

(2.54)

A simpler form of this equation can be obtained by using transformations \( \tilde{E} = [\star \epsilon]^{\frac{1}{2}} E \) and \( \tilde{B} = [\star \mu^{-1}]^{\frac{1}{2}} B \). Please note here that these transformations are valid for inhomogeneous media with positive permittivity and permeability values, and with the cell-based (face-based in 2-D) material definitions since this results in a symmetric positive semi-definite Hodge matrices, \([\star \epsilon]\) and \([\star \mu^{-1}]\). After the transformations, it reads as

\[
\begin{bmatrix}
    \tilde{E}^n \\
    \tilde{B}^{n+\frac{1}{2}}
\end{bmatrix} =
\begin{bmatrix}
    I & \Delta t C^T \\
    -\Delta t C & I - \Delta t^2 C C^T
\end{bmatrix}
\begin{bmatrix}
    \tilde{E}^{n-1} \\
    \tilde{B}^{n-\frac{1}{2}}
\end{bmatrix}
\]

(2.55)
where

\[ C = [\star_{\mu-1}]^{\frac{1}{2}}[D_{\text{curl}}^*][\star_\epsilon]^{-\frac{1}{2}} \]  

(2.56)

2.5.2 System matrix for semi-discrete update equations

In order to complete the stability analysis of the system in (2.55), additional constraints are required. This is done by relating the discrete system in (2.55) to the semi-discrete system of (2.8)-(2.9). Augmenting \( \mathcal{E} \) and \( \mathcal{B} \) in these equations give

\[ j\omega \begin{bmatrix} \mathcal{E} \\ \mathcal{B} \end{bmatrix} = \begin{bmatrix} 0 & \mathcal{E}^{-1}[D_{\text{curl}}^*][\star_{\mu-1}] \\ -[D_{\text{curl}}] & 0 \end{bmatrix} \begin{bmatrix} \mathcal{E} \\ \mathcal{B} \end{bmatrix} \]  

(2.57)

Transformations \( \mathcal{E}' = [\star_\epsilon]^{\frac{1}{2}}\mathcal{E} \), \( \mathcal{B}' = [\star_{\mu-1}]^{\frac{1}{2}}\mathcal{B} \), which has been applied in the previous section for the discrete update equations can also be applied here. The transformed equations read as

\[ j\omega \begin{bmatrix} \mathcal{E}' \\ \mathcal{B}' \end{bmatrix} = \begin{bmatrix} 0 & C^T \\ -C & 0 \end{bmatrix} \begin{bmatrix} \mathcal{E}' \\ \mathcal{B}' \end{bmatrix} \]  

(2.58)

Eqn. (2.58) is in the form of eigenvalue decomposition with purely imaginary eigenvalues \( j\omega \) and eigenvectors \( \mathcal{E}' \) and \( \mathcal{B}' \). Denoting an arbitrary eigenvector associated with this system as \([\bar{e}_\omega^T, \bar{b}_\omega^T]^T\), this equation can also be written more explicitly as

\[ C^T\bar{b}_\omega = j\omega \bar{e}_\omega \]  

(2.59)

\[ -C\bar{e}_\omega = j\omega \bar{b}_\omega \]  

(2.60)

2.5.3 Stability criterion

In order to relate the above finding, (2.59)-(2.60) to the discrete system equations, the following particular form of eigenvectors is assumed for the discrete system

\[ \bar{x} = \begin{bmatrix} \alpha \bar{e}_\omega \\ \bar{b}_\omega \end{bmatrix} \]  

(2.61)
where $\alpha$ is a complex-valued constant. Testing this vector as the eigenvector of the matrix in (2.55) with eigenvalue $\lambda$ gives

$$
\begin{bmatrix}
I & \Delta t C^T \\
-\Delta t C & I - \Delta t^2 CC^T
\end{bmatrix}
\begin{bmatrix}
\alpha \bar{e}_\omega \\
\bar{b}_\omega
\end{bmatrix}
= \lambda
\begin{bmatrix}
\alpha \bar{e}_\omega \\
\bar{b}_\omega
\end{bmatrix}
$$

(2.62)

Performing the matrix-vector multiplication on the left-hand side in (2.62) and substituting (2.59)-(2.60) produces

$$
\begin{bmatrix}
(\alpha - j\omega \Delta t) \bar{e}_\omega \\
(1 - \alpha j\omega \Delta t + \Delta t^2 (j\omega)^2) \bar{b}_\omega
\end{bmatrix}
= \lambda
\begin{bmatrix}
\alpha \bar{e}_\omega \\
\bar{b}_\omega
\end{bmatrix}
$$

(2.63)

After eliminating $\bar{e}_\omega$ and $\bar{b}_\omega$ by multiplying individual equation lines, $\alpha$ can be found as

$$
\alpha = \frac{\Delta t j\omega}{2} \pm \sqrt{\left(\frac{\Delta t j\omega}{2}\right)^2 + 1}
$$

(2.64)

Eigenvalue $\lambda$ associated with $\alpha$ can be found by substituting the above expression of $\alpha$ back in the second line of (2.63). It reads as

$$
\lambda = 1 - \frac{(\Delta t \omega)^2}{2} \pm j(\Delta t \omega) \sqrt{1 - \frac{(\Delta t \omega)^2}{4}}
$$

(2.65)

Stability of the system in (2.55) is related to magnitude of the eigenvalue $\lambda$, which can be written after derivations as

$$
|\lambda| = \begin{cases} 
1, & \text{if } (\Delta t \omega)^2 \leq 4, \\
1 - \frac{(\Delta t \omega)^2}{2} \pm (\Delta t \omega) \sqrt{\frac{(\Delta t \omega)^2}{4} - 1}, & \text{if } (\Delta t \omega)^2 > 4.
\end{cases}
$$

(2.66)

Magnitude of the eigenvalues show two different type of behaviors for two conditions listed in (2.66). For $(\Delta t \omega)^2 \leq 4$, magnitude of the eigenvalues is less than or equal to 1, whereas in the remaining region two eigenvalues appear with one smaller than 1, and the other greater than 1. Since stability requires all eigenvalues inside the unit-circle, $|\lambda| < 1$, stability criterion for FETD can be written as

$$
\Delta t < \frac{2}{\max(\omega)} \text{, for } \forall \omega
$$

(2.67)
where the exact value of \( \max(\omega) \) depends on the properties of the particular mesh and material constants. In practice, this value is not easily accessible and time step is chosen according to length of the shortest edge of the mesh, \( l_{\text{min}} \), and it is given by \( \Delta t = c_N l_{\text{min}} / v_c \). A conservative value for the Courant number is \( c_N = 0.2 \). Please note that in the presence of permittivity and permeability values different from that of free space, appropriate adjustments need to be performed to \( v_c \) in the above expression.

We note here however that, one needs to take special care of the singularity that occurs in \( \alpha \) in (2.64) when \( \lambda = 0 \). This case corresponds to static modes with eigenvectors of form \( [\bar{e}^T_\omega, \bar{0}]^T \). It is easy to verify that this expression is an eigenvector of (2.58) with \( \lambda = 0 \), therefore these static forms also form an orthonormal set.

The second requirement for stability of the method is to have a linearly independent set of eigenvectors. Since the system matrix of the semi-discrete equations described in (2.58) is anti-symmetric, it is well-known that the associated eigenvectors form a full orthonormal set [72]. Therefore eigenvectors of the discrete equations which are given as a linear transformation of the eigenvectors of semi-discrete equations, (2.61), also form a linearly independent set. This can be shown as follows. If we denote the matrix composed of columns of eigenvectors that correspond to a particular eigenvalue \( \lambda \) for the discrete and semi-discrete equations as \( \bar{V}_\alpha \) and \( \bar{T}_\alpha \) respectively, rank of \( \bar{V}_\alpha \) and \( \bar{T}_\alpha \) can be related as
\[
\text{rank}(\bar{T}_\alpha) = \text{rank} \left( \begin{bmatrix}
\bar{e}_0 & \bar{e}_1 & \ldots & \bar{e}_{N_\alpha} \\
\bar{b}_0 & \bar{b}_1 & \ldots & \bar{b}_{N_\alpha}
\end{bmatrix} \right) \quad (2.68)
\]
\[
= \text{rank} \left( \begin{bmatrix}
\bar{e}_0 & \bar{e}_1 & \ldots & \bar{e}_{N_\alpha} \\
\bar{b}_0 & \bar{b}_1 & \ldots & \bar{b}_{N_\alpha}
\end{bmatrix} \right) \quad (2.69)
\]
\[
= \text{rank}(\bar{V}_\alpha) \quad (2.70)
\]

Therefore since eigenvectors of the semi-discrete system is orthonormal and linearly independent, eigenvectors of the discrete system that share the same eigenvalue, \(\bar{V}_\alpha\), are also linearly independent. It can be further concluded that since eigenvectors associated with different eigenvalues are linearly independent by the nature of eigenvalue decomposition, all eigenvectors of the discrete system are found linearly independent.

As a result, the \(E-B\) FETD is stable for inhomogeneous media with symmetric positive definite Hodge matrices as long as the length of the time step is below a certain value as described in (2.67).

### 2.6 Late-time stability and energy conservation

Numerical stability and energy conservation properties of the proposed finite element time-domain algorithm are tested for \(10^7\) time steps. We consider a 31.4286 × 31.4286 m cavity with perfect electrical conducting walls and with a source wavelength \(\lambda_0 = 30\) m, and \(\epsilon_x(k) = \epsilon_y(k) = \epsilon_0, \mu_z(k) = \mu_0\). The point source is located at the center of the computational domain. The discrete energy is given by

\[
W = E^T[\ast_\epsilon]E + B^T[\ast_{\mu^{-1}}]B 
\quad (2.71)
\]

We plot \(W\) as a function of time (in a temporal log scale) in Fig. 2.9 to verify the energy conserving characteristic of the mixed finite element time-domain method. The
inset of Fig. 2.9 shows the time history of the magnetic field sampled at \( x_{rec} = 15 \) m and \( y_{rec} = 10 \) m, for two different scenarios: (a) air-filled cavity (same scenario of the energy conservation test), (b) cavity backed by an 8-cells perfectly matched layer and filled with lossy dispersive material (San Antonio clay loam). The field values are normalized by the peak field value in scenario (a). Due to losses in the dispersive material and in the perfectly matched layer, the magnetic field exhibit a decay in time for scenario (ii) until it reaches the numerical noise floor. Note that the increase in the ripple frequency at late times is just an artifact from the temporal log scale. We note here that the stability observed in the numerical test cases is only an indication for the late-time stability and a proof requires a more thorough analysis of the method.

2.7 Concluding remarks

We have described a \( E-B \) mixed finite element time-domain method to simulate Maxwell equations in inhomogeneous and doubly-dispersive linear media. The proposed method provides a more straightforward approach to incorporate complex frequency dispersive characteristics simultaneously in the permittivity and in the permeability because it factors out the update of Maxwell curl equations (involving the spatial derivatives) from the update of the constitutive equations. When combined with a leap-frog time integration scheme, the resulting algorithm is shown to be late-time stable and, in lossless media, energy-conserving (symplectic). The final finite element time-domain update equations have a form somewhat similar to that of the finite-difference time-domain update equations in (doubly-)dispersive media, except
Figure 2.9: Discrete energy as a function of time inside a rectangular cavity, showing that the algorithm is energy-conserving. The inset shows the normalized magnetic field at the probe location for two different scenarios: (a) air-filled cavity (no energy dissipation) and (b) cavity filled by (lossy) dispersive and backed by a perfectly matched layer. The increase in the ripple frequency seen at late times is an artifact stemming from the log scale used for the time steps.
for the sparse linear solve required in the electric field update equation. Perfectly matched layers can also be included in a simple fashion.
Absorbing boundary conditions are routinely employed in FDTD and FETD simulations of open-domain problems in order to avoid spurious reflections from the grid terminations. The perfectly matched layer (PML) in particular has become a very popular absorbing boundary condition because of its efficacy and ease of implementation, and because it preserves the underlying sparsity of the methods. The PML was originally developed for rectangular FDTD grids (Cartesian PML) [83–88] and later implemented in rectangular FETD grid terminations [51, 80, 89, 90].

The original PML concept applied only to Cartesian coordinates (planar interfaces). To extend its range of applicability, the PML concept was implemented in nonorthogonal FDTD grids and curvilinear FEM meshes with good results [91–93]. However, these implementations were based on an approximate matching because they assumed of the metric coefficients to be independent of the spatial coordinates, which is not true in curvilinear coordinates. Later, true PMLs – in the sense of providing reflectionless absorption in the continuum limit – were derived for cylindrical and spherical mesh terminations in [94–98]. and, more generally, for conformal mesh terminations in [31, 99] based on a complex stretching (analytic continuation) of the normal coordinate to the mesh termination [100].
A conformal PML is of interest because it can be placed on the convex hull enclosing the scatterer(s) to reduce the amount of buffer space in the computational domain. The savings in memory can be considerable, especially in problems involving impenetrable scatterer(s), as illustrated in Fig. 3.1. The conformal PML can be expressed in terms of dispersive and anisotropic constitutive tensors that depend on the local principal radii of curvature of the mesh termination surface [99]. Implementations of the conformal PML have been considered in non-staggered body-fitted FDTD grids [101, 102], frequency-domain finite element simulations [103–106], and FETD simulations [107], the latter being restricted to the second-order wave equation FETD formulation.

Figure 3.1: A conformal PML (left) can greatly reduce the amount of buffer space around the scatterer compared to the Cartesian PML (right).
In this study, we develop a conformal PML implementation for the mixed $E$-$B$ FETD algorithm [14]. As alluded above, the mixed FETD algorithm provides a simple and natural route to incorporate the dispersive and anisotropic tensors that comprise the conformal PML since the update of the constitutive equations is derived and implemented separately from the update of Maxwell curl equations. Indeed, in the mixed FETD, the conformal PML implementation boils down to a modification in the calculation of the two Hodge (mass) matrices $[\star_\epsilon]$ and $[\star_{\mu-1}]$.

The proposed conformal PML-FETD formulation is tested in a number of examples involving transient field scattering from both impenetrable (PEC) and penetrable (dispersive media) objects, to verify its efficacy. The late-time stability of the conformal PML and the energy conservation properties of the underlying FETD are also verified numerically.

### 3.1 Formulation

The permittivity and permeability tensors of the conformal PML in the TE$_z$ case are given in terms of the stretching variables $\gamma(\rho)$ and $s(\rho)$ in local coordinates indicated in Fig. 3.2 as follows [99, 101]

\[
\begin{align*}
\bar{\epsilon}(\vec{r}) &= \bar{\epsilon}(\rho) = \hat{\rho} \hat{\rho} \frac{\gamma(\rho)}{\gamma(\rho)} + \hat{\psi} \hat{\psi} \frac{s(\rho)}{\gamma(\rho)} \\
\bar{\mu}(\vec{r}) &= \bar{\mu}(\rho) = \hat{\zeta} \hat{\zeta} \gamma(\rho) s(\rho)
\end{align*}
\]  

(3.1)

where

\[
\begin{align*}
\gamma(\rho) &= \frac{1}{\rho} \left( \rho_0 + \int_{\rho_0}^{\rho_0+l} s(\rho) d\rho \right) = \kappa(\rho) + \frac{\sigma(\rho)}{j \omega \epsilon_0} \\
s(\rho) &= 1 + \frac{\sigma(\rho)}{j \omega \epsilon_0}
\end{align*}
\]  

(3.2)  

(3.3)
The point $\vec{r}$ along the radial direction inside the PML is given in terms of the local coordinate $\rho$ as $\vec{r} = \rho \hat{\rho} = (\rho_0 + l) \hat{\rho}$, as illustrated. Note that the coordinate system depicted here is a local one, with the (local) radius of curvature $\rho_0$ at the free-space/PML boundary being a function of the point $M$ along the PML interface [99].

A local (z-invariant) orthogonal Darboux frame [99] with unit vectors $\hat{\rho}$, $\hat{\phi}$, and $\hat{z}$ is utilized in (3.1)-(3.3). This is locally equivalent to a cylindrical coordinate system with the origin located at the (local) center of curvature of each point $M$ along the PML interface [99], cf. Fig. 3.2.

In 2-D, a face-based discretization for the PML tensors is used with $\bar{\epsilon}(\rho)$ indexed as $\bar{\epsilon}(k)$ and $\bar{\mu}(\rho)$ indexed as $\bar{\mu}(k)$, where $k$ is the face index. The PML parameters can be similarly indexed as $\gamma(k)$, $s(k)$, $\sigma_\rho(k)$, $\sigma_\phi(k)$, and $\kappa(k)$.

### 3.1.1 Electric field update

In order to obtain the electric field update, a set of algebraic manipulations are performed on the Hodge matrix $[\star \epsilon]$. If we denote face $k$ as $\Omega_k$, the domain of
integration in (2.6) can be decomposed as a sum over the $\Omega_k$’s so that

$$[\star \epsilon]_{ij} = \sum_{k=1}^{N_f} \int_{\Omega_k} \vec{W}_i^1 \cdot \vec{\epsilon}(k) \cdot \vec{W}_j^1 \, d\Omega$$

(3.4)

Substituting (3.1) in (3.4) and separating components yields

$$[\star \epsilon] = \sum_{k=1}^{N_f} \frac{\gamma(k)}{s(k)} [\mathcal{L}_\rho(k)] + \sum_{k=1}^{N_f} \frac{s(k)}{\gamma(k)} [\mathcal{L}_\phi(k)]$$

(3.5)

with $[\mathcal{L}_\rho(k)]_{ij}$ given by

$$[\mathcal{L}_\rho(k)]_{ij} = \int_{\Omega_k} \left( \hat{\rho} \cdot \vec{W}_i^1 \right) \left( \hat{\rho} \cdot \vec{W}_j^1 \right) \, d\Omega$$

(3.6)

and similarly for $[\mathcal{L}_\phi(k)]_{ij}$. A further simplification can be performed by considering the Hodge matrix-vector multiplication in (2.10) and defining an electric flux density vector$^2$ $\mathbb{D} = [\star \epsilon] \mathbb{E}$. Substituting (3.5) in this definition for $\mathbb{D}$, we get

$$\mathbb{D} = \sum_{k=1}^{N_f} \frac{\gamma(k)}{s(k)} [\mathcal{L}_\rho(k)] \mathbb{E} + \sum_{k=1}^{N_f} \frac{s(k)}{\gamma(k)} [\mathcal{L}_\phi(k)] \mathbb{E}$$

(3.7)

Although the above summations run over all faces, the inner-products $[\mathcal{L}_\rho(k)]$ and $[\mathcal{L}_\phi(k)]$ produce non-zero values only for two faces per edge. If we denote these faces as $k_{ij}$ and $k_{ij}^+$ for each edge $j$, and denote $\mathbb{D} = [d_1, d_2, \ldots, d_{N_f}]^T$, the summation above can be rewritten as

$$d_j = \sum_{i=1}^{N_e} \frac{s(k_{ij})}{\gamma(k_{ij})} [\mathcal{L}_\rho(k_{ij})]_{ij} e_i + \sum_{i=1}^{N_e} \frac{\gamma(k_{ij})}{s(k_{ij})} [\mathcal{L}_\rho(k_{ij})]_{ij} e_i$$

$$+ \sum_{i=1}^{N_e} \frac{s(k_{ij})}{\gamma(k_{ij})} [\mathcal{L}_\phi(k_{ij})]_{ij} e_i + \sum_{i=1}^{N_e} \frac{\gamma(k_{ij})}{s(k_{ij})} [\mathcal{L}_\phi(k_{ij})]_{ij} e_i$$

(3.8)

$^2$Note that, inside the PML, the electric flux density defined in this manner incorporates PML stretching variables.
Each term in (3.8) can be considered separately, by taking the stretching variables out of the summation and writing

\[ d_j = d_{\rho j} + d_{\varphi j} + d_{\varphi^1 j} + d_{\varphi^1 j} \]  \hspace{1cm} (3.9)

where

\[ d_{\rho j} = \gamma(k_{\rho j}) \frac{e_{\rho j}}{s(k_{\rho j})} \]  \hspace{1cm} (3.10)

and

\[ e_{\rho j} = \sum_{i=1}^{N_e} \mathcal{L}_\rho(k_{\rho j})_{ij} e_i \]  \hspace{1cm} (3.11)

and similarly for \( d_{\varphi j}, d_{\varphi^1 j}, e_{\varphi j}, e_{\varphi^1 j}, \) and \( e_{\varphi^1 j}, \) with \( j = 1, \ldots, N_e. \) Note that four different equations per edge need to be considered because each edge touches two faces and each face possibly has two different frequency dependencies (along \( \varphi \) and \( \rho \)). Substituting (3.2) and (3.3) into (3.10) and rearranging terms, \( d_{\rho j} \) and \( e_{\rho j} \) can be related through

\[ d_{\rho j} = \frac{\sigma_\varphi(k) + j\omega_0 \kappa(k)}{\sigma_\rho(k) + j\omega_0} e_{\rho j} \]  \hspace{1cm} (3.12)

The time-domain discretization of (3.12) is inverse Fourier transforming and approximating time derivatives using central differences with time step \( \Delta t. \) The resulting update equation is given by

\[ d_{\rho j}^{n+1} = \left( \frac{\sigma_\varphi(k_{\rho j}) \Delta t + 2\epsilon_0 \kappa(k_{\rho j})}{\sigma_\rho(k_{\rho j}) \Delta t + 2\epsilon_0} \right) e_{\rho j}^{n+1} \]

\[ + \left( \frac{\sigma_\varphi(k_{\rho j}) \Delta t - 2\epsilon_0 \kappa(k_{\rho j})}{\sigma_\rho(k_{\rho j}) \Delta t + 2\epsilon_0} \right) e_{\rho j}^n \]

\[ - \left( \frac{\sigma_\rho(k_{\rho j}) \Delta t - 2\epsilon_0}{\sigma_\rho(k_{\rho j}) \Delta t + 2\epsilon_0} \right) d_{\rho j}^n \]  \hspace{1cm} (3.13)
and similarly for \( d_{\rho|i} \), \( d_{\varphi|i} \), \( d_{\varphi|i} \). If we denote the factor multiplying \( e^{\rho_{ij}|n+1} \) in the above equation as \( w_{\rho}(k_{ij}) \) and the overall contribution from the (known) past time step field values as \( g_{\rho|j}|n \), (3.13) can be written more compactly as

\[
d_{\rho|j}|^{n+1} = w_{\rho}(k_{ij})e^{\rho_{ij}|n+1} + g_{\rho|j}|^{n}
\]  

Substituting (3.11), (3.14), and the corresponding expressions for \( d_{\rho|i} \), \( d_{\varphi|i} \), \( d_{\varphi|i} \) in (3.9), and writing the result in a matrix form, we obtain

\[
[\mathcal{A}]\mathbb{E}^{n+1} = \mathbb{D}^{n+1} - \mathbb{G}^{n}
\]  

where

\[
[\mathcal{A}] = [\mathcal{W}_\rho][\mathcal{L}_\rho] + [\mathcal{W}_\rho][\mathcal{L}_\varphi] + [\mathcal{W}_\varphi][\mathcal{L}_\rho] + [\mathcal{W}_\varphi][\mathcal{L}_\varphi]
\]  

with \( [\mathcal{W}_\rho] = \text{diag}\{w_{\rho}(k_{i1}), w_{\rho}(k_{i2}), \ldots, w_{\rho}(k_{iN_e})\} \) and similarly for \( [\mathcal{W}_\rho] \), \( [\mathcal{W}_\varphi] \), \( [\mathcal{W}_\varphi] \), and \( \mathbb{G} = [g_1, g_2, \ldots, g_{N_e}]^T \) with \( g_j = g_{\rho|j} + g_{\rho|j} + g_{\varphi|j} + g_{\varphi|j} \).

### 3.1.2 Magnetic field update

The magnetic field update can be derived along similar lines as the electric field update. The final update equation for the magnetic field is written in matrix form as

\[
[\mathcal{A}_\mu]\mathbb{H}^{n+\frac{1}{2}} = \mathbb{B}^{n+\frac{1}{2}} - \mathbb{G}_\mu^{n-\frac{1}{2}}
\]  

where \([\mathcal{A}_\mu]\) and \(\mathbb{G}_\mu^n\) are analogous to \([\mathcal{A}]\) and \(\mathbb{G}^n\) respectively. The column vector \(\mathbb{H} = [\star_{\mu-1}]\mathbb{B}\) represents magnetic field intensity. The matrix \([\mathcal{A}_\mu]\) is defined as the diagonal matrix given by the matrix product

\[
[\mathcal{A}_\mu] = [\mathcal{W}_z][\mathcal{L}_z]
\]
where $[L_z]$ and $[W_z]$ are both diagonal matrices representing inner-product and coefficient matrices analogous to $[L_\rho]_{ij}$ and $[W_\rho]$, respectively. Since $[A_\rho]$ is diagonal (explicit update), no linear solve is required in the magnetic update.

### 3.1.3 Curl equations and full update

The update equations for $\mathbf{D}$ and $\mathbf{B}$ are explicit and can be obtained directly from a leap-frog time discretization of (2.8) and (2.9) with $\mathbf{D} = [\star_z] \mathbf{E}$ as

\begin{align}
\mathbf{D}^{n+1} &= \mathbf{D}^n + \Delta t [\nabla_{\text{curl}}]^T \mathbf{H}^{n+\frac{1}{2}} - \Delta t \mathbf{J}_s^{n+\frac{1}{2}} \\
\mathbf{B}^{n+\frac{1}{2}} &= \mathbf{B}^{n-\frac{1}{2}} - \Delta t [\nabla_{\text{curl}}] \mathbf{E}^n - \Delta t \mathbf{M}_s^n
\end{align}

A complete time step update for the electromagnetic fields consists of applying (3.20), (3.17), (3.19), and (3.15) in sequence.

For the 3-D implementation, two basic changes are necessary in the development above. First, the tensor in (3.1) should be replaced by the more general tensor derived in [99], in terms of the two principal radii of curvature of a general (doubly-curved) surface. This would produce three terms, instead of two in (3.5) and (3.7). Second, since an edge contacts more than two faces in 3-D, extra terms would appear in (3.8).

### 3.2 Results

The accuracy of the proposed PML-FETD is examined via several test cases. Unless specified otherwise, the common parameters used in the following examples are as follows. TE$_z$ problems are considered in 2-D with an magnetic point source excited by an ultra-wideband (UWB) time-domain excitation of the form $f(t) = -0.488 \sin(2\pi v_c/\lambda_0) + 0.290 \sin(4\pi v_c/\lambda_0) - 0.031 \sin(6\pi v_c/\lambda_0)$ for $0 < t < \lambda_0/v_c$ and $f(t) = 0$ otherwise (a Blackman-Harris pulse derivative), where $v_c$ is the speed of light.
The central wavelength in free space is \( \lambda_0 = 0.6 \) m, which corresponds to a central frequency of 500 MHz. The time step is chosen according to the length of the shortest edge \( l_{\text{min}} \) and is given by \( \Delta t = c_N l_{\text{min}}/v_c \), with Courant number \( c_N = 0.2 \). A mesh generation algorithm with a maximum face element area constraint \( \Omega_k < \sqrt{3} l_e^2/4 \) for all faces \( k = 1, \ldots, N_f \), is used, where \( l_e \) is the resolution of the mesh in terms of an edge length. A sparse incomplete Cholesky factorization with a drop tolerance value \( 10^{-10} \) is used to solve (3.15). The shape of the PML boundary is described by analytical functions, while the radius of curvature required in the calculation of the conformal PML parameters is calculated numerically using a set of grid points much denser than the finite-element nodes. This implies that the error in the (numerical) calculation of the local radius of curvature is negligible vis-à-vis other sources of error. A polynomial profile of order \( m = 2.5 \) is used for the PML stretching variable \( s(\rho) \). The maximum value of the PML conductivity profile is determined by the standard criterion used for FDTD [1].

### 3.2.1 Scattering from a PEC circular cylinder

In this section, the scattered field from a PEC circular cylinder is calculated using the conformal PML-FETD and compared against both FDTD and analytical results. The center of the cylinder is located at \((x_o, y_o) = (0.4, 0.4) \) m and the cylinder has a radius \( R = 0.34 \) m. An average edge length of \( \lambda/60 = 1 \) cm is used for the finite element mesh, which is shown in Fig. 3.3(a). The source is located at \((x_s, y_s) = (0.96, 0.45) \) m and the magnetic field is probed at \((x_p, y_p) = (0.96, 0.35) \) m. The scattered field is given by \( s_{kp}|^n = h_{kp}^c|^n - h_{kp}^f|^n \), where \( h_{kp}^c|^n \) is the magnetic field calculated with circular cylinder present and \( h_{kp}^f|^n \) is the magnetic field calculated
in free-space. The number of (rectangular) faces in the reference FDTD simulation is chosen the same as the number of faces in the FETD simulation. A staircase approximation is used to model the circular cylinder in FDTD.

The analytical solution is obtained from the Green’s function for this problem, which is expressed in terms of a Hankel-Bessel series over the azimuth index [54, pp. 574-667], with the first 50 terms included. The time-domain source excitation is first converted to frequency-domain by a Fourier transformation. The frequency resolution is increased by zero padding with a length that is 10 times the total number of time steps. The source spectrum, at each frequency, is multiplied by the analytical solution at that frequency. The final time-domain result is obtained by an inverse Fourier transformation.

Fig. 3.3(b) shows that the scattered field obtained by the conformal PML-FETD agrees very well with both FDTD and analytical results. The normalized residual error in FETD is calculated as

$$\delta(n) = 20 \log_{10} \left( \frac{f_{\text{etd}}^n - s_{\text{analytic}}^n}{\max_n s_{\text{analytic}}^n} \right)$$

and similarly for FDTD. The residual error is shown in Fig. 3.3(c). It is seen that the error in the FDTD result is larger than the FETD error for the resolution considered, with peak levels of $-44\text{dB}$ and $-28\text{dB}$ for FETD and FDTD, respectively. This is despite the fact that the edge length in the FDTD grid is smaller than the average edge length of the FETD grid (0.77 cm versus 1.00 cm).

### 3.2.2 Conformal PML: Reflection error

The accuracy of the proposed conformal PML is further demonstrated by calculating reflection errors using different number of layers $N_{PML}$ in the PML region. In this
Figure 3.3: Scattered field and normalized residual error for a point source illuminating a circular PEC cylinder. (a) The finite element mesh comprises 33,487 edges and 22,046 faces. The source and the probe location are located at the right of the scatterer, indicated by small + and × symbols, respectively. (b) The time-domain response of the conformal PML-FETD method and the FDTD method agree very well with the analytical result. (c) Due to staircasing approximations, the error in the FDTD result is on average about 10 dB larger than the error in the FETD result for the mesh considered.
case, an oval-shaped computational domain with size $0.6 \times 1.2$ m$^2$ is extruded with $N_{PML} = 4, 8, 16, 24$. The finite element mesh for $N_{PML} = 8$ is depicted in the inset of Fig. 3.4. The average edge length is chosen as $\lambda_0/60 = 1$ cm. The reflection error as a function of time is obtained by placing the point source at $(x_s, y_s) = (0.3, 0.4)$ m and probing the field at $(x_p, y_p) = (0.3, 0.5)$ m. In order to estimate the reflection error as function of position along the conformal PML boundary, the source and probe locations are chosen at different points along the computational domain both at a distance 6 cm away from the PML boundary and 4 cm away from each other. A FETD simulation with the same mesh extruded by an appropriate larger number of \textit{free-space} layers (so that the spurious reflection can be windowed out from the results) is used as reference. The extruded part of the mesh (corresponding to PML or free-space) consists of convex quadrilateral tiles composed of two triangular faces each. These tiles are orthogonal in the Darboux frame local coordinates $\rho$ and $\varphi$ [99]. A separate reference result consisting of the same mesh terminated by a PEC boundary (and with no extrusion) is used to normalize the reflection coefficient. If we denote the magnetic field values at the probe locations in the simulations with the PML mesh, free-space extruded mesh and the PEC-terminated mesh as $h_{k_p}^{\text{pml}}|n|$, $h_{k_p}^f|n|$ and $h_{k_p}^\text{pec}|n|$, where $n$ is the time step index, the reflection error is calculated as follows

$$R_{PML}(n) = 20 \log_{10} \left( \frac{|h_{k_p}^{\text{pml}}|n| - h_{k_p}^f|n||}{\max_n |h_{k_p}^\text{pec}|n| - h_{k_p}^f|n||} \right)$$ (3.22)

Fig. 3.4 shows the reflection errors with respect to time and angular position along the PML boundary for different $N_{PML}$. The angular axis in Fig. 3.4(b) refers to the location of the source-probe pair in a cylindrical coordinates system centered at $(x_c, y_c) = (0.3, 0.6)$ m. Fig. 3.4 clearly shows that $R_{PML}$ decreases as $N_{PML}$ is
Figure 3.4: Reflection error vs. (a) time and (b) position along the PML boundary, for various $N_{PML}$: (a) The PML reflection levels are progressively reduced for larger $N_{PML}$, with $R = -68\,\text{dB}$ obtained for $N_{PML} = 24$. (b) The PML reflection errors peak at $90^\circ$, where the radius of curvature is minimum because a smaller radius reduces the average distance of nearby PML boundary points to the probe location. The finite-element mesh used in this example has 12,748 edges and 8,428 faces.
increased with peak reflection levels of $-49\text{dB}$ and $-68\text{dB}$ are observed for $N_{PML} = 8$ and $N_{PML} = 24$, respectively. Fig. 3.4(b) shows that the reflection errors peaks at $90^\circ$. This is because the smaller radius of curvature at that angle reduces the average distance of nearby PML boundary points to the probe location.

The convergence of $R_{PML}$ with respect to $N_{PML}$ is slower in this FETD implementation than what is observed in typical FDTD simulations. The slow convergence of PML in FETD versus FDTD has also been observed elsewhere [13,80]. Since those papers are based on rectangular PML, it suggests that such feature is related to the finite-element method itself, rather than to conformality aspects. The discretization of the PML conductivity profile is one of the major sources of PML reflection error and one important difference of FETD in this regard is that it does not posses the staggered nature of the FDTD grid. Staggering allows for FDTD to effectively assign twice the number of PML conductivity jumps: one set at electric field locations and the other set at magnetic field locations. This error can be mitigated by using a relatively fine mesh resolution. In this example, we employ on average 60 edges per (central) wavelength. However, there is a fundamental trade-off here because an increase in the mesh resolution—for a given $N_{PML}$—reduces the overall PML thickness and hence the overall attenuation within it.

### 3.2.3 Conformal PML: Parameter study

In order to analyze the performance of the conformal PML, finite-element mesh depicted in Fig. 3.4(b) is used. The average edge length is chosen as $\lambda_0/30 = 1 \text{ cm}$. The reflection error as a function of time is obtained at two different locations; point A: $(x_p, y_p) = (23.07, 41.24) \text{ m}$ with the source at $(x_s, y_s) = (23.81, 39.37) \text{ m}$, and point
B: \((x_p, y_p) = (13.92, 55.36)\) m with the source at \((x_s, y_s) = (15.90, 55.62)\) m. Note here that points A and B are in the vicinity of a PML interface section with small and large radii of curvature, respectively. At each location, a source-receiver pair is placed 6 cm away from the PML interface and 4 cm away from each other.

A polynomial profile with maximum conductivity \(\sigma_{max}\) and polynomial coefficient \(M\) is used in the PML region. The profile is given as \(\sigma_{p}(k) = \sigma_{max}(l/d)^M\), where \(d\) is the total width of PML and \(l\) is the distance between the layer associated with face \(k\) and the PML interface.

The reflection error \(\Gamma = R_{PML}(n)\) in time at both location A and B for \(N_{pml} = 12\), \(\sigma_{max} = 0.5\sigma_{opt}\) and \(M = 2\) is shown in Fig. 3.5. The maximum error observed at location A is found to be approximately 10 dB higher than the error at location B, mainly due to the difference in the radius of curvature associated with these points. For instance, it can be seen from Fig. 3.4(b) that, location A is in the vicinity of PML with small radius of curvature and larger faces, which increases the numerical dispersion at this point. It can also be seen from the figure that the error levels are lower than a finite-difference time-domain (FDTD) simulation with similar parameters. One possible explanation is that the face-based material definition in the finite-element method assigns only one material step at each PML layer, as opposed to two in (staggered grid) FDTD.

Fig. 3.6 shows the reflection error at both locations for \(N_{pml} = 16\) with respect to normalized maximum conductivity \((\sigma_{max}/\sigma_{opt})\), where \(\sigma_{opt} = (M + 1)/(150\pi \sqrt{\varepsilon_0} l_p)\) is the optimum value used for FDTD, and the PML grading polynomial coefficient \(M\). It can be seen from the figure that the reflection error at location A is 15 dB higher than that at B due to lower radius of curvature. The optimum value for maximum
conductivity is observed to be approximately half of $\sigma_{opt}$. Again, this may be due to the face-based material definition in the finite-element method which assigns a single material step per layer, as opposed to one in FDTD. This increases the error due to conductivity steps and requires a slightly smoother profile for a given $N_{pml}$ or $M$.

Fig. 3.7 shows the reflection error at both locations with respect to number of PML and several different $M$. The error follows the theoretical reflection values of PML and converges rapidly for $N_{pml} < 7$. The speed of convergence is reduced for larger number of layers, where it is dominated by a separate error mechanism possibly related to the numerical dispersion error associated with the higher frequency range of the source spectrum.
Figure 3.6: Reflection error at locations A and B with respect to normalized maximum conductivity and PML grading polynomial coefficient ($N_{pml} = 16$). Optimum maximum conductivity is observed to be half of FDTD optimum value, $\sigma_{opt}$.
Figure 3.7: Reflection error at locations A and B with respect to number of layers and the PML grading polynomial coefficient ($\sigma_{max}/\sigma_{opt} = 0.5$).
3.2.4 Scattering from oval PEC coated with metamaterial

Although the basic formulation presented in Section 3.1 corresponds to free-space, it is easy to extend the mixed E-B FETD to media having inhomogeneous frequency-dependent tensors $\bar{\epsilon}(\vec{r}, \omega)$ and $\bar{\mu}(\vec{r}, \omega)$, as detailed in [13].

In this Section, the scattered field from an oval-shaped PEC scatterer coated with a doubly-dispersive isotropic metamaterial layer as shown in Fig. 3.8(a) is considered. The mesh for this example has average edge lengths of 1 cm and 0.3227 cm in the free space and metamaterial regions, respectively. The mesh shown in Fig. 3.8(a) has 28,556 edges and 18,741 faces. This is approximately 1.9 times less than would be required using a Cartesian PML for the same problem. The frequency response of the metamaterial layer is described by a two-species Debye model for both the permittivity and the permeability. The permittivity model writes as

$$\epsilon(\omega) = \epsilon_0 \epsilon_\infty + \epsilon_0 \sum_{i=1}^{2} \frac{A^\epsilon_i}{1 + j\omega \tau^\epsilon_i}$$

with parameters given by $\epsilon_\infty = 3.0$, $A^\epsilon_1 = 1.45$, $A^\epsilon_2 = 0.35$, $\tau^\epsilon_1 = 1.5$ nsec, $\tau^\epsilon_2 = 0.25$ nsec, and $\sigma = 1.0$ mS/m. The two-species Debye model for the permeability has parameters $\mu_\infty = 1.0$, $A^\mu_1 = 0.35$, $A^\mu_2 = 0.65$, $\tau^\mu_1 = 2.0$ nsec, $\tau^\mu_2 = 0.1$ nsec. The source is located at $(x_s, y_s) = (0.8, 0.34)$ m and the probe at $(x_p, y_p) = (0.78, 0.16)$ m.

Fig. 3.8(b) shows the scattered fields obtained by the conformal PML-FETD, compared to a reference FDTD result using Cartesian PML, showing very good agreement.

3.2.5 Monostatic-RCS: Ogive cylinder

We next calculate the monostatic radar cross-section (RCS) of an ogive-shaped PEC object with a geometrical singularity as depicted in Fig. 3.9(a). The mesh shown in Fig. 3.9(a) has 103,367 edges and 67,881 faces. A mesh of similar density
Figure 3.8: (a) Finite element mesh for an oval-shaped PEC scatterer coated with a doubly-dispersive material. The mesh has 28,556 edges and 18,741 faces. The source and the probe are located at the right of the scatterer and indicated by small + and × symbols, respectively. A Cartesian PML implementation for this problem would require a mesh about 1.9 times larger. (b) Scattered fields calculated by FETD and FDTD, showing very good agreement.
employing a Cartesian PML would require approximately 230,000 edges and 150,000 faces, more than twice the size of the mesh using the conformal PML. RCS calculations for similar geometries were studied using a Cartesian PML-FETD based on the second order wave equation in [89,90].

For the RCS calculation, a plane-wave excitation is realized following a methodology similar to the plane-wave injection described in [1, pp. 201-212]. The scattered field is transformed to the frequency domain and the far-field is obtained by using a near- to far-field transformation. These operations are carried out at a contour in the tiled portion of the mesh that would normally separate different layers of the PML region. The PML stretching however, is offset by three layers in this case so that both the plane wave excitation and the near- to far-field transformation are done in the free-space region. The plane wave is injected through equivalent electric and magnetic source terms $J_s(\vec{r}) = \hat{n} \times \vec{H}_i(\vec{r})$ and $M_s(\vec{r}) = -\hat{n} \times \vec{E}_i(\vec{r})$, where $\hat{n}$ is the outward unit vector normal to the injection contour at $\vec{r}$. The magnetic field vector associated with the plane-wave excitation is given in the time-domain by

$$\vec{H}_i(\vec{r}, t) = \hat{z} f(t - t_0 - \hat{\beta}_i \cdot \hat{r} / v_c)$$

(3.24)

where $\hat{\beta}_i = \hat{x} \cos \varphi_i + \hat{y} \sin \varphi_i$ is the unit vector for incidence angle $\varphi_i$. The parameter $t_0$ is simply a time-offset for the FETD pulse excitation so that all fields in the computational domain are equal to zero for $t \leq 0$. The time-domain excitation $f(t)$ is again the Blackman-Harris pulse derivative. The contour comprised of edges that separate the tiled and non-tiled regions of the mesh (original PML boundary that is now offset by three layers) is used to insert the electric current source. The magnetic current source is applied at the two faces that touch each of these edges (with equal weights). The near- to far-field transformation is applied at a contour.
two cells away from the plane wave injection contour. In 2-D, the RCS is calculated using the following expression

\[
RCS(\varphi) = \left| \frac{\int_\mathcal{C} \left[ P(\vec{r}) - Q(\vec{r}) \right] e^{\beta \hat{r} \cdot \vec{r}} \, dl'}{4 |\beta| |F(\omega)|^2} \right|^2
\]

(3.25)

with

\[
P(\vec{r}) = \beta \hat{z} \times (\hat{n} \times \vec{H}_s(\vec{r})) \cdot \hat{r}
\]

(3.26)

\[
Q(\vec{r}) = \omega \epsilon_0 \hat{z} \cdot (\hat{n} \times \vec{E}_s(\vec{r}))
\]

(3.27)

where \( \beta = \omega / v_c \) is the wavenumber, \( \mathcal{C} \) denotes the near-to-far field transformation contour, \( dl' \) is the infinitesimal arclength along \( \mathcal{C} \), \( \vec{E}_s(\vec{r}) \) and \( \vec{H}_s(\vec{r}) \) are the frequency-domain scattered electric and magnetic fields evaluated along \( \mathcal{C} \), \( F(\omega) \) is the Fourier transform of \( f(t) \), and \( \hat{r} = \hat{x} \cos \varphi + \hat{y} \sin \varphi \) is the unit vector pointing towards the observation point. The lengths of the major and minor axes of the ogive are \( 8\lambda \) and \( 1\lambda \), respectively. The average edge length of the finite element mesh is chosen as \( 0.015\lambda \).

Fig. 3.9 shows the monostatic RCS calculated by the conformal PML-FETD, compared against frequency-domain finite element results and method of moments (MoM) results [109], showing again very good agreement.

### 3.2.6 Late-time stability and energy conservation

For a time-domain method based on a leap-frog update, there are necessary conditions on the matrices \([D_{\text{curl}}], [D_{\text{curl}}^*], [\epsilon], \) and \([\mu^{-1}]\) for (conditional) stability and energy conservation to hold, as discussed, e.g., in [73]. In order to numerically demonstrate late-time stability and energy conservation here, a scenario with the same
Figure 3.9: (a) The finite element mesh used to calculate the monostatic RCS of the ogive cylinder has 103,367 edges and 67,881 faces. A Cartesian PML implementation for this problem would require a mesh about 2.3 times larger. (b) Monostatic RCS of the ogive with size $4\lambda_0 \times 1\lambda_0$ calculated by FETD, frequency-domain finite elements, and method of moments (MoM) [109].
domain boundary shape of Fig. 3.4(b) but scaled down four times (for faster update) is used (the average edge length is kept the same). The source is placed at \((x_s, y_s) = (0.1, 0.07)\) m and the magnetic field is probed at \((x_s, y_s) = (0.1, 0.13)\) m. Stability is tested by considering two different cases: (i) a cavity problem simulated by a mesh extruded by eight layers of free-space directly terminated by a PEC boundary, and (ii) a cavity problem simulated by the same mesh but where now the eight extruded layers constitute the PML. The total number of steps used in both cases is \(10^7\). The discrete energy is calculated by

\[
W = \mathbf{E}^T [\varepsilon] \mathbf{E} + \mathbf{B}^T [\mu_{r-1}] \mathbf{B}
\]  

(3.28)

Fig. 3.10 shows the discrete energy with respect to time in the PEC-backed cavity problem where it is clearly seen that energy is conserved. Note that the increase in the oscillations is just an artifact of the logarithm scale chosen for the abscissa. The inset of Fig. 3.10 shows the time history of the magnetic field magnitude at the probe location. After \(10^7\) time steps, the magnetic field magnitude in the PML-backed case is about \(-150\) dB down from that in the PEC-backed problem due to PML losses. The very small residual field value that remains is comprised of high-frequency components (with wavelength close to the average edge length) that are not well absorbed by the PML. No late-time instabilities or spurious linear growth \([80,81]\) are observed.

It should be pointed out that a conformal PML cannot be deployed over grid terminations having convex portions as viewed from inside the computational domain (i.e., with negative local radius of curvature under the present convention). In that case, the conformal PML would exhibit a dynamically unstable behavior. This is discussed in some detail elsewhere \([102,110]\).
Figure 3.10: The main plot shows the discrete energy for $10^7$ time steps inside an oval shaped cavity terminated by PEC. The energy is constant except for small periodic fluctuations due to the leap-frog approximation in the time integration. This shows the energy-conserving property of the proposed method. The inset shows the normalized magnetic field magnitude in the PEC- and PML-backed cavity simulations, showing the late-time stability of the PML.
3.3 Concluding remarks

We have developed and implemented a conformal PML absorbing boundary condition for the FETD simulation of transient Maxwell equations in open-domain problems. The underlying FETD algorithm is based on a (mixed) expansion of the electric field in terms of edge elements and of the magnetic field in terms of face elements. The time discretization employs a leap-frog time update akin to FDTD except for a linear solve required for the electric field update.

The conformal PML produces significant computational savings by minimizing the buffer space in the computational grid around the scatterer(s). The accuracy and capabilities of the conformal PML-FETD have been demonstrated through several examples involving PEC scatterers and (doubly-)dispersive materials. The late-time stability and energy conservation properties of the method have also been verified numerically.
CHAPTER 4

FDTD-FETD HYBRIDIZATION IN INHOMOGENEOUS DISPERSIVE MEDIA

Although FDTD has simple and explicit update equations and well-known numerical properties, it is based on a regular structured grid with limited geometrical flexibility. In order to alleviate this problem, several extensions have been introduced, such as curvilinear implementation [111, 112], locally conformal implementation [113–117], subgridding [6–11, 118–122], etc. Although these extensions listed here can produce significant improvements, most of them target specific type of problems. They are also known to possess certain limitations and difficulties of their own.

Finite-element time-domain (FETD) is based on a unstructured mesh [2] and offers higher geometrical flexibility. Although FETD can accurately solve problems with complex geometry, it is also known to be highly computationally intensive due to implicit nature of the update equations. The efficiency of the method for a fixed discretization can be improved by using preconditioners, reordering methods or iterative solution methods [123].

A compromise methodology is to hybridize FDTD and FETD [124–141]. In this strategy, part of domain with detailed features are modeled by an unstructured mesh and updated via FETD, whereas the remaining part is modeled by rectangular cells
and updated by FDTD. This produces an algorithm that simultaneously takes advantage of the relatively efficient nature of the FDTD updates and geometrical flexibility of FETD.

Since these methods are, in general, based on different type of cells and time-integration, spatial and temporal interfacing needs to be performed for communicating FDTD and FETD portions of the mesh. In earlier methods this has been accomplished by a general overlapping methodology and spatial interpolation [126,128–131]. These methods allow one to interface separate meshes without any geometrical arrangement specific to interfacing. However they are also known to produce complications based on interpolations such as instabilities. As an alternative, hybrid method can be based on a single mesh consisting of heterogeneous element types including hexahedral cells of FDTD [127,132], [135–141]. This leads to a natural hybridization, since FDTD can be expressed as a specific FETD implementation with mass lumping on the mass matrices [135]. Although a two-dimensional implementation can be only based on triangular and rectangular elements, a three-dimensional implementation requires additional elements for geometric interfacing. Pyramidal element [15–17] features the smallest number of edges and faces when compared to other possible element types and it has been widely used for this purpose [135–141].

Finite-element part of the hybrid method has so far been based on the second-order wave equation on the electric or magnetic fields, and a time-integration based on the second derivative [124–141]. On the other hand, FDTD is based on the first-order coupled Maxwell’s equation and a leap-frog time-integration. Due to this incompatibility, in the current hybrid implementations, special care needs to be taken in
choosing the specific time-integration method for FETD to ensure stability of the hybrid method [136].

In this section, a hybrid FDTD-FETD algorithm based on the \( E-B \) mixed vector FETD method will be studied. Due to dependence of the FETD part on the first order coupled Maxwell’s equations and a leap-frog update, the update equations for the \( E-B \) mixed vector FETD method, (2.10)-(2.11), closely resemble the update equations for FDTD. Moreover, it has also been shown that by choosing rectangular (roof-top) basis functions and performing lumping on the mass matrix, FDTD can be expressed as a specific implementation of \( E-B \) mixed vector FETD. Therefore these two methods constitute a better choice for hybridization when compared to existing hybridization methodologies which are based on the second-order Maxwell’s equations. Moreover, as mentioned in section 2.2, the constitutive equations are decoupled from the curl equations producing a straightforward implementation for frequency-dispersive media. In particular implementation of doubly-dispersive tensors is considered in this study.

In this section, implementation of the hybrid FDTD-FETD method scheme is described. The efficiency and accuracy is also demonstrated through numerical examples in 2-D and 3-D.

4.1 General formulation

In this formulation a three dimensional mesh consisting of a combination of tetrahedral, cubical, and pyramidal elements is considered. Since a transition from the tetrahedral to cubical portions of the mesh is not geometrically possible, pyramidal elements are used in the interfaces of these two element types [15–17]. However note
that the formulation presented here is also valid in meshes with pyramidal elements utilized elsewhere. Among the alternative pyramidal element definitions that have been proposed, a compatible-element is chosen for this study [17]. This particular element preserves the favorable characteristics of the $E$-$B$ mixed vector FETD method.

In order to perform the hybridization, the cells of the composite mesh are first grouped into two sets: (i) FETD update cells, \( \{e_i, b_k\} \in U_{fetd} \), and (ii) FDTD update cells, \( \{e_i, b_k\} \in U_{fdd} \). Cells which belong to at least one tetrahedral or pyramidal element are placed in the FETD update set, \( U_{fetd} \). All the remaining cells are placed in the FDTD update set \( U_{fdd} \). Since both methods are based on a leap-frog discretization, the overall update equation is a straightforward combination of the FETD update equations and the FDTD update equations with a common time step \( \Delta t \). Following section describes the update equations for FETD.

### 4.2 Finite-element update

Update equations for FETD consists of generalization of those that was presented in section 2.2 to 3-D. A cell-based material definition is chosen, where the material profile within each cell is assumed constant, i.e., \( \overline{\varepsilon}(\vec{r}) \rightarrow \overline{\varepsilon}(k) \) and \( \overline{\mu}(\vec{r}) \rightarrow \overline{\mu}(k) \), where \( k \) is the cell index. Unlike implementations based on other material definitions available such as face or edge definitions, this results in a symmetric matrix solution.

Inhomogeneous and dispersive material tensors for a 3-D problem in Cartesian coordinates are given as

\[
\overline{\varepsilon}(k; \omega) = \hat{x}\hat{x} \varepsilon_x(k; \omega) + \hat{y}\hat{y} \varepsilon_y(k; \omega) + \hat{z}\hat{z} \varepsilon_z(k; \omega) \\
\overline{\mu}(k; \omega) = \hat{x}\hat{x} \mu_x(k; \omega) + \hat{y}\hat{y} \mu_y(k; \omega) + \hat{z}\hat{z} \mu_z(k; \omega)
\] (4.1) (4.2)
with

\[
\epsilon_x(k; \omega) = \frac{\sum_{p=0}^{N_p} q_x^{(p)}(k) (j_\omega)^p}{\sum_{p=0}^{N_p} r_x^{(p)}(k) (j_\omega)^p}
\] (4.3)

and similarly for \(\epsilon_y(k; \omega)\), \(\epsilon_z(k; \omega)\), \(\mu_x(k; \omega)\), \(\mu_y(k; \omega)\) and \(\mu_z(k; \omega)\).

### 4.2.1 Electric field constitutive equation update

In this section \(\mathbb{D}\) in (2.3) is decomposed in a form suitable for time-discretization. If we denote \(N_c\) and \(\Omega_k\) as number of cells and the volume of the \(k\)th cell respectively, (2.3) can be rewritten as a sum of cell contributions as

\[
[\star \epsilon]_{ij} = \sum_{k=1}^{N_c} \int_{\Omega_k} \tilde{W}_i^1 \cdot \tilde{\epsilon}(k) \cdot \tilde{W}_j^1 \, d\Omega 
\] (4.4)

Substituting (4.1) into (4.4) and separating terms for each of three axis components yields

\[
[\star \epsilon]_{ij} = \sum_{k=1}^{N_c} \int_{\Omega_k} \epsilon_x(k) \left( \hat{x} \cdot \tilde{W}_i^1 \right) \left( \hat{x} \cdot \tilde{W}_j^1 \right) \, d\Omega \\
+ \sum_{k=1}^{N_c} \int_{\Omega_k} \epsilon_y(k) \left( \hat{y} \cdot \tilde{W}_i^1 \right) \left( \hat{y} \cdot \tilde{W}_j^1 \right) \, d\Omega \\
+ \sum_{k=1}^{N_c} \int_{\Omega_k} \epsilon_z(k) \left( \hat{z} \cdot \tilde{W}_i^1 \right) \left( \hat{z} \cdot \tilde{W}_j^1 \right) \, d\Omega 
\] (4.5)

By using the fact that material tensors are assumed uniform within each cell, it is possible to further simplify (4.5) as

\[
[\star \epsilon] = \sum_{k=1}^{N_c} \epsilon_x(k) \mathbb{L}_x(k) + \sum_{k=1}^{N_c} \epsilon_y(k) \mathbb{L}_y(k) + \sum_{k=1}^{N_c} \epsilon_z(k) \mathbb{L}_z(k) 
\] (4.6)
with

$$[L_x(k)]_{ij} = \int \limits_{\Omega_k} (\hat{x} \cdot \hat{W}_{i}^-) (\hat{x} \cdot \hat{W}_{j}^-) \, d\Omega$$

(4.7)

and similarly for $[L_y(k)]_{ij}$ and $[L_z(k)]_{ij}$. Constitutive relation based on the simplified expression for the hodge matrix (2.3) is obtained by substituting (4.6) into (2.3). It can be written as

$$D = \sum_{k=1}^{N_c} \epsilon_x(k) [L_x(k)]E + \sum_{k=1}^{N_c} \epsilon_y(k) [L_y(k)]E + \sum_{k=1}^{N_c} \epsilon_z(k) [L_z(k)]E$$

(4.8)

Although the summation above includes all $k$ cells, the inner-product integrals $[L_x(k)]_{ij}$, $[L_y(k)]_{ij}$ and $[L_z(k)]_{ij}$ are non-zero only for the cells that touch edge $j$. If $M_c(j)$ denotes the number of cells that touch edge $j$, and $k_{mj}$ as the $m$th cell that touches edge $j$, each element $d_j$ of the array $D$ can be written as

$$d_j = \sum_{m=1}^{M_c(j)} \sum_{i=1}^{N_e} \epsilon_x(k_{mj}) [L_x(k_{mj})]_{ij} e_i + \sum_{m=1}^{M_c(j)} \sum_{i=1}^{N_e} \epsilon_y(k_{mj}) [L_y(k_{mj})]_{ij} e_i + \sum_{m=1}^{M_c(j)} \sum_{i=1}^{N_e} \epsilon_z(k_{mj}) [L_z(k_{mj})]_{ij} e_i$$

(4.9)

We can further write

$$d_j = \sum_{m=1}^{M_c(j)} \left( d_{x mj} + d_{y mj} + d_{z mj} \right)$$

(4.10)

where

$$d_{x mj} = \epsilon_x(k_{mj}) e_{x mj}$$

(4.11)

and

$$e_{x mj} = \sum_{i=1}^{N_e} [L_x(k_{mj})]_{ij} e_i$$

(4.12)
and similarly for \( d_{ymj}, d_{zmj}, e_{ymj}, \) and \( e_{zmj} \) with \( j = 1, \ldots, N_e \).

It is observed from (4.10) that \( 3M_e(j) \) functions are required in the update of a single edge, as opposed to 6 in the 2-D implementation, and a single one in a FDTD implementation. This comes from the fact that each edge contacts \( M_e(j) \) different cells with possibly different dispersion characteristics in each of three dimensions. Note that significant algorithmic reductions in this number can be obtained by omitting the separation of terms that share the same material tensor on an edge-by-edge basis.

The ordinary differential equation that is obtained from (4.11) in time-domain can be solved by using similar steps to (2.24)-(2.27) producing the auxiliary vectors \( \mathcal{D}_{xm} \) and \( \mathcal{G}_{xm} \). Note here that since number of terms required for each edge is different, these vectors are composed by using the available elements, \( d_{xmj} \) and \( g_{xmj} \), whenever possible. Zeros are used in the remaining positions in the vectors. This produces \( M_e = \max_j M_e(j) \) vectors per each axis direction.

Similar to (2.28), update equation for the auxiliary electric flux is obtained as

\[
\mathcal{D}_{xm}^{n+1} = [\mathcal{W}_{xm}] [\mathcal{L}_{xm}] \mathcal{E}^{n+1} + \mathcal{G}_{xm}^n
\]  

(4.13)

where \([\mathcal{L}_{xm}]_{ij} = [\mathcal{L}_x(k_{mj})]_{ij}\) and \([\mathcal{W}_{xm}] = \text{diag}\{w_x(k_{m1}), w_x(k_{m2}), \ldots, w_x(k_{mN_e})\}\), and similarly for \( \mathcal{D}_{ym}^{n+1} \) and \( \mathcal{D}_{zm}^{n+1} \). From (4.10) we can write

\[
\mathcal{D} = \sum_{m=1}^{M_e} (\mathcal{D}_{xm} + \mathcal{D}_{ym} + \mathcal{D}_{zm})
\]  

(4.14)

Substituting (4.13) in (4.14) the final update equation for \( \mathcal{E} \) can be written as

\[
[\mathcal{A}] \mathcal{E}^{n+1} = \mathcal{D}^{n+1} - \mathcal{G}^n
\]  

(4.15)
where

\[
[A] = \sum_{m=1}^{M_e} \left( [\mathcal{W}_{xm}] [\mathcal{L}_{xm}] + [\mathcal{W}_{ym}] [\mathcal{L}_{ym}] + [\mathcal{W}_{zm}] [\mathcal{L}_{zm}] \right) \quad (4.16)
\]

### 4.2.2 Magnetic field constitutive equation update

Following the derivations for the electric field update, the mass matrix for permeability, \([\mathbf{x}_{\mu^{-1}}]_{ij}\) can be written as

\[
[\mathbf{x}_{\mu^{-1}}]_{ij} = \sum_{k=1}^{N_e} \mu_x^{-1}(k) [\mathcal{L}_x(k)]_{ij} + \sum_{k=1}^{N_e} \mu_y^{-1}(k) [\mathcal{L}_y(k)]_{ij} + \sum_{k=1}^{N_e} \mu_z^{-1}(k) [\mathcal{L}_z(k)]_{ij} \quad (4.17)
\]

with

\[
[\mathcal{L}_x(k)]_{ij} = \int_{\Omega_k} \left( \hat{x} \cdot \vec{W}_i^2 \right) \left( \hat{x} \cdot \vec{W}_j^2 \right) d\Omega \quad (4.18)
\]

and similarly for \([\mathcal{L}_y(k)]_{ij}\) and \([\mathcal{L}_z(k)]_{ij}\).

Update equations for \(\mathbb{H}\) are derived similarly to \(\mathbb{E}\). The main difference is that since a face contacts up to two faces, only \(M_\mu = 2\) dispersive terms needs to be used in contrast to the electric field update which uses \(M_e\) terms. Following similar steps to those in (4.8)-(4.16), the update equation for \(\mathbb{H}\) can be found as

\[
\mathbb{H}^{n+1} = [A_{\mu^{-1}}] \left( \mathbb{B}^{n+1} - \mathcal{G}_{mu}^n \right) \quad (4.19)
\]

where

\[
[A_{\mu^{-1}}] = \sum_{m=1}^{2} \left( [\mathcal{W}_{xim}] [\mathcal{L}_{xm}] + [\mathcal{W}_{yim}] [\mathcal{L}_{ym}] + [\mathcal{W}_{zim}] [\mathcal{L}_{zm}] \right) \quad (4.20)
\]

Curl-equations for the 3-D \(E-B\) mixed vector FETD implementation is same with the update equations in 2-D, given in (2.38)-(2.39).
4.3 Finite-difference update

For the FDTD portion of the mesh, an Auxiliary-Differential-Equation (ADE) [1] implementation is used. In this implementation derivatives of the electric field and electric flux density is used as auxiliary variables. FDTD grid axis directions are assumed to be aligned with the \( x, y \) and \( z \) directions without loss of generality. The update for the \( E_x \) field is given as follows

\[
D^{n+1}_{x(i+\frac{1}{2},j,k)} = D^n_{x(i+\frac{1}{2},j,k)} + \frac{\Delta t}{\varepsilon} \left( \frac{H^{n+\frac{1}{2}}_{x(i+\frac{1}{2},j+\frac{1}{2},k)} - H^{n+\frac{1}{2}}_{x(i+\frac{1}{2},j-\frac{1}{2},k)}}{\Delta y} \right. \\
\left. - \frac{H^{n+\frac{1}{2}}_{y(i+\frac{1}{2},j+\frac{1}{2},k)} - H^{n+\frac{1}{2}}_{y(i+\frac{1}{2},j-\frac{1}{2},k)}}{\Delta z} \right)
\]

(4.21)

\[
E^{n+1}_{x(i+\frac{1}{2},j,k)} = \frac{1}{w_x(i+\frac{1}{2},j,k)} \left( D^{n+1}_{x(i+\frac{1}{2},j,k)} + \sum_{p=0}^{N_p} v^{(p)}_{x(i+\frac{1}{2},j,k)} E^{(p)}_{x(i+\frac{1}{2},j,k)} \right. \\
\left. - \sum_{p=0}^{N_p} u^{(p)}_{x(i+\frac{1}{2},j,k)} D^{(p)}_{x(i+\frac{1}{2},j,k)} \right)
\]

(4.22)

where \( E^{n+1}_{x(i+\frac{1}{2},j,k)} \) and \( D^{n+1}_{x(i+\frac{1}{2},j,k)} \) are electric field intensity and electric flux density, respectively; \( E^{(p)}_{x(i+\frac{1}{2},j,k)} \) and \( D^{(p)}_{x(i+\frac{1}{2},j,k)} \) are auxiliary vectors representing the \( p \)th derivative of \( E_x \) and \( D_x \); \( w^{(p)}_{x(i+\frac{1}{2},j,k)} \), \( v^{(p)}_{x(i+\frac{1}{2},j,k)} \) and \( u^{(p)}_{x(i+\frac{1}{2},j,k)} \) are constants for the ADE implementation at location \((i + \frac{1}{2}, j, k)\) defined in Appendix A.

4.4 Numerical results

The accuracy and efficiency of the proposed scheme is tested via several numerical examples in two and three dimensions. In the two-dimensional examples, a mesh-generator with maximum area constraint \( \Omega_k < \sqrt{3}l_e^2/4 \) for all elements \( k \) is used, where \( l_e \) is the mesh resolution in terms of an edge length. Problems consist of a
rectangular domain and a soft magnetic line source. In three-dimensional examples, a mesh-generator with maximum volume constraint $\Omega_k < \sqrt{2}l_c^3/12$ for all elements $k$ is used. In this case, a cubical domain shape and $z$-directed soft magnetic point source is chosen. In all problems, side-length of the FDTD cells is chosen as $s = 0.7l_c$. The time-domain excitation is given by $f(t) = -0.488 \sin(2t\pi v_c/\lambda_0) + 0.290 \sin(4t\pi v_c/\lambda_0) - 0.031 \sin(6t\pi v_c/\lambda_0)$ for $0 < t < \lambda_0/v_c$ and $f(t) = 0$ otherwise (Blackman-Harris pulse derivative), where $\lambda_0$ is the free-space wavelength associated with the central frequency, and $v_c$ is the speed of light. When applicable, linear interpolation is used to perform excitation at a specified point in the mesh. Same procedure is used for obtaining the field values from the mesh. The time step is chosen according to length of the shortest edge of the mesh, $l_{\text{min}}$, and given by $\Delta t = c_N l_{\text{min}}/v_c$. The Courant number is chosen as $c_N = 0.2$. A sparse incomplete Cholesky factorization with a drop tolerance value $10^{-10}$ and $10^{-6}$ is used for solving (2.30) and (4.15), respectively. An iterative symmetric MLQ (a conjugate-gradient variant) decomposition with drop tolerance value $10^{-3}$ is also used in large 3D problems.

### 4.4.1 Validation: Cylindrical scatterer

In order to demonstrate the accuracy and efficiency of the proposed scheme in 2-D, transmitted fields in a cylinder filled with dispersive material in free-space is compared with the results of three alternative methods that are illustrated in Fig. 4.1. A broadband soft magnetic source with a Blackmann-Harris driving function is placed at $(x_s, y_s) = (-5, 15)$ cm. The transmitted field is observed at location $(x_p, y_p) = (5, 5)$ cm. The following two-pole Debye model is used to model both permittivity and permeability.
\[ \epsilon_x(\omega) = \epsilon_y(\omega) = \epsilon_0\epsilon_\infty + \epsilon_0 \sum_{i=1}^{2} \frac{A_i^\epsilon}{1 + j\omega \tau_i^\epsilon} \]  

(4.23)

with the parameters for permittivity given by \( \epsilon_\infty = 2.0, A_1^\epsilon = 2.35, A_2^\epsilon = 0.55, \)
\( \tau_1^\epsilon = 1.20 \text{ nsec}, \tau_2^\epsilon = 0.60 \text{ nsec and } \mu = \mu_0. \) Parameters for permeability are based
on the same two-pole Debye model with \( \mu_\infty = 1.0, A_1^\mu = 0.40, A_2^\mu = 0.10, \tau_1^\mu = 0.30 \)
nsec and \( \tau_2^\mu = 1.40 \text{ nsec}. \)

Fig. 4.4.1 shows that the transmitted magnetic fields for the hybrid methods
match with alternative methods and proposed method can successfully simulate a
cylinder with dispersive material. Furthermore, a comparison of Fig. 4.1(a) and
4.1(d) suggests that; even though a larger number of cells are used to resolve the fields
inside and outside the cylinder in the finite-difference simulation, a lower accuracy is
observed when compared to the full-hybrid simulation. Since the numerical dispersion
error is expected to be higher in the latter, this is attributed to the improvement in
the geometrical modeling of the cylinder in the finite-element simulation.

In order to demonstrate the accuracy of the method in 3-D, a problem with a
cubical cavity with z-directed magnetic point source excitation is considered. The
source is located at \((x_s, y_s)=(-0.8,0,0) \text{ m and the probe at (0.8,0,0) m with the origin}
located in the center of a cubical computational domain with size 1.7 \times 1.7 \times 1.7
m. Cavity is filled with either free-space or a doubly-dispersive material with the
model in (4.23) and parameters \( \epsilon_\infty = 2.666, A_1^\epsilon = 1.667, A_2^\epsilon = 0.482, \tau_1^\epsilon = 5.714 \)
nsec, \( \tau_2^\epsilon = 10.48 \text{ nsec, } \mu = \mu_0, \mu_\infty = 1.0, A_1^\mu = 0.563, A_2^\mu = 0.435, \tau_1^\mu = 20.0 \)
nsec and \( \tau_2^\mu = 7.142 \text{ nsec. The computational domain is discretized by cubical cells}
except for a patch of size 0.3 \times 0.3 \text{ m located at the center of the computational}
domain which contains tetrahedral and pyramidal elements. Central wavelength of
Figure 4.1: Meshes used in the Hybrid FETD-FDTD simulations. Number of rectangular (□) and triangular (△) elements used are indicated in captions of subfigures.
Figure 4.2: (a) Transmitted fields inside a cylindrical scatterer for different methods that are illustrated in Fig. 4.1. (b) Normalized residual error in the transmitted fields. Hybrid method accuracy matches similar methods with less number of triangular elements and thus with a smaller matrix problem to solve at each time-step. FDTD produces larger errors mainly due to geometrical modeling errors although three times higher resolution is used.
the excitation is chosen as $\lambda_0 = 6 \text{ m}$ and $\lambda_0 = 10 \text{ m}$ in free space and dispersive problems respectively. Mesh resolution is chosen as $l_e = 0.1429 \text{ m}$ with side-length of the cubical cells equal to $a_c = 0.1 \text{ m}$. Analytical solution is obtained by utilizing the Green’s function associated with the problem in free-space [54, pp. 545, 646] and spectral representation of the source excitation. Green’s function for the cavity problem is constructed by superposing appropriate images of the free-space Green’s function with respect to the cavity walls [54, pp. 317]. In order to increase the frequency resolution, zero-padding by $\times 30$ and $\times 2000$ the original length, is applied to the source excitation for the free-space and doubly-dispersive cases respectively. The larger length used in the latter is to capture the fast frequency variation of the dispersive material profile. Fig. 4.3 shows the total fields and residual errors with respect to the analytical solution.

It can be seen in Fig. 4.3 that transient response obtained for both free-space and doubly-dispersive cases match the analytical result. An initial error level of -45 dB is obtained in the free-space simulation with a monotonic increase in later time-steps. The increase is mainly due to accumulation of numerical dispersion errors. In the doubly-dispersive case a similar -45 dB initial error level is obtained. However due to the losses in the dispersive material profile, a decrease is observed in the magnetic field magnitude and the associated error. Error in the hybrid simulation is observed to be 8 dB higher when compared to the mixed-element FETD on the average. This is due to the increased numerical dispersion error of FDTD when compared to FETD on the same mesh.
Figure 4.3: Magnetic fields and normalized residual errors for the transient response of a point source in a 3-D cubical cavity problem. Initial error level of -45 dB is obtained in both problems. The increase and decrease of the error levels in (a) and (b) in later time steps can be attributed to numerical dispersion and losses, respectively. Hybrid method produces 8 dB larger errors when compared to mixed-element FETD, due to higher numerical dispersion errors in the FDTD portion of the grid.
4.4.2 Residual error

Due to change in the numerical dispersion characteristics and the transition from implicit to explicit update, interface between FDTD and FETD portions of the mesh produce spurious reflections. In this section, reflection error for different mesh resolutions are studied in 2-D. A linear interface in a PEC-terminated free-space domain that is large enough to contain the excited wave-field up to the maximum desired time-step is used. Source is located \( d_s = 0.10 \) m away from the interface in the FDTD portion of the domain, whereas probe is located \( d_p = 0.05 \) m away from the interface in the FETD portion. The central-wavelength of the source is chosen as \( \lambda_0 = 0.4 \) m. Fig. 4.4 shows the reflection error for different resolutions.

Figure 4.4: Residual error in transmitted field for a problem with planar hybrid interface for different resolution values. Error can be reduced down to -57 dB for \( l_e = 0.005 = \lambda_0/80 \).
It can be seen from Fig. 4.4 that the error can be reduced down to -57 dB for \( l_e = 0.005 = \lambda_0/80 \).

**4.4.3 Material traverse hybrid interface**

In order to demonstrate the accuracy for a case with material traversing the hybrid interface in 3-D, a cavity with size 2.7 \( \times \) 1.7 \( \times \) 1.7 m\(^3\), partially filled with doubly dispersive material for \( y > 0.9 \) is considered. A \( z \)-sireded broadband soft magnetic source with a Blackmann-Harris driving function with \( \lambda_0 = 12 \) m is placed at \((x_s, y_s, z_s) = (0.05, 0.85, 0.80) \) cm with the origin located at one of the corners of the cavity. The transmitted magnetic field, \( H_z \), is observed at location \((x_p, y_p, z_p) = (3.65, 0.85, 0.80) \) cm. Size of the cells in the FDTD portion of the domain is chosen as 0.1 \( \times \) 0.1 \( \times \) 0.1 m\(^3\). Material parameters for the dispersive media is chosen same with that used in the 3-D example in section 4.4.1. In the hybrid method, tetrahedral region is located at the center of the cavity with size 2.3 \( \times \) 0.3 \( \times \) 0.3 m\(^3\), so that region with the dispersive media traverses the hybrid interface. Fig. 4.5 compares the transmitted magnetic field in the hybrid case with that in a case with FDTD. In order to eliminate the effect of numerical dispersion and isolate errors due to interfacing, same cell size is used in both cases.

It can be observed from Fig. 4.5 that a considerable match is observed in between hybrid and FDTD results. Therefore no considerable discrepancies are produced in the illustrated case where a material traverses the hybrid interface.

**4.4.4 Stability tests in free-space**

The proof that was provided in section 2.6 for the FETD method can be directly generalized to the hybrid method. The only requirement is the symmetric positive
Figure 4.5: Transmitted magnetic fields at the probe location for a cavity partially filled with doubly-dispersive material. Hybrid interface traversing the material interface does not introduce any significant discrepancies.
definiteness of the Hodge matrices, which is satisfied for the hybrid method by con-
struction of the Hodge matrices. Nonetheless, a numerical analysis for stability of
the hybrid method in free-space is performed in both 2-D and 3-D by analyzing the
eigenvalues and eigenvectors associated with the system matrix for a small problem.
The associated mesh and mesh cross-section are depicted in insets of Figs. 4.6 and
4.7 for 2-D and 3-D respectively. In order to calculate the system matrix, (2.10) is
substituted in (2.11) and it is augmented with (2.11) as follows

\[
\bar{M} = \begin{bmatrix}
I & \Delta t[D_{\text{curl}}]^{-1}D_{\text{curl}}^T[\star_{\mu^{-1}}] \\
-\Delta t[D_{\text{curl}}] & I - \Delta t^2[\star_{\epsilon}]^{-1}D_{\text{curl}}^T[\star_{\mu^{-1}}]
\end{bmatrix}
\begin{bmatrix}
E^{n-1} \\
H^{n-\frac{1}{2}}
\end{bmatrix}
\] (4.24)

Figs. 4.6 and 4.7 shows the eigenvalues of the system matrix, \(\bar{M}\) for the 2-D
and 3-D problems, respectively. Mixed-element FETD method results associated
with the same meshes are also included as references in both problems. Moreover,
further analysis revealed that the eigenvectors associated with multiple eigenvalues
are linearly independent. Hence, stability of the proposed hybrid scheme in free-space
is demonstrated.

### 4.4.5 PML performance

In this section PML performance is calculated in a 3-D problem for both the hybrid
method and the mixed-element FETD method. A rectangular domain consisting of
cubical elements with dimensions 2.3 \(\times\) 2.3 \(\times\) 2.3 m is used with a patch of size
0.3 \(\times\) 0.3 \(\times\) 0.3 m at the center composed of tetrahedral and pyramidal elements.
Resolution of the mesh is chosen as \(a_c = 0.1m\), where \(a_c\) is the side-length of cubes
and rectangular faces of the pyramids. A source excitation with \(\Lambda_0 = 2.0\) is applied
to the center of the patch at \((x_s, y_s) = (1.15, 1.15)\) m. z-component of the magnetic
Figure 4.6: Eigenvalues of the system matrix for the mixed-FETD and hybrid FDTD-FETD methods in 2-D. The mesh used in both methods is shown in inset of (a). The mesh consists of 237 nodes, 520 edges and 284 faces. Eigenvalues are on the unit circle with the maximum discrepancy in the order of numerical noise, $\delta < -280 \text{ dB}$. Eigenvectors associated with multiple-eigenvalues are found linearly independent.
Figure 4.7: Eigenvalues of the system matrix for the mixed-FETD and hybrid FDTD-FETD methods in 3-D. The cross-section of the mesh used in both methods is shown in inset of (a). The mesh consists of 530 nodes, 1425 edges, 1338 faces and 424 cells. Eigenvalues are on the unit circle with the maximum discrepancy in the order of numerical noise, $\delta < -280$ dB. Eigenvectors associated with multiple-eigenvalues are found linearly independent.
field is observed at \((x_p, y_p) = (0.1, 0.1)\) m. Computational domain is extended by layers made up of cubical cells in cases with PML. As the reference, a simulation with similar extension is used. In this case an appropriate (large) number of free-space layers are used in the place of PML. If we denote \(h_{krec}^{pml}\) and \(h_{krec}^{ref}\) as the magnetic field z-component obtained from the PML simulation and the reference simulation, respectively, the normalized reflection error is calculated by

\[
R_{pml}(n) = 20 \log_{10} \left( \frac{|h_{krec}^{pml}|_n - |h_{krec}^{ref}|_n}{\max_n |h_{krec}^{ref}|_n} \right) \tag{4.25}
\]

Fig. 4.8 shows the normalized reflection errors for the hybrid-FETD and mixed-element FETD methods. Error levels of -54 dB and -79 dB are observed in mixed-element FETD and hybrid FDTD-FETD methods, respectively. Low error levels in the hybrid method can be explained as follows: The performance of PML in hybrid FDTD-FETD is mainly based on that of FDTD method, since PML regions in the proposed method is assigned to FDTD. In this case PML profile is discretized both on the faces and edges of the cubes with a total number of \(2N_{pml}\) steps for \(N_{pml}\) layers. The performance in the mixed-element FETD however, is based on the FETD PML performance which is based on a cell-based material profile. In this case only \(N_{pml}\) profile steps are used, lowering the accuracy of the PML significantly. We would like to note here that although the choice of cell-based materials in the FETD method results in symmetric hodge matrices, a disadvantage in PML performance results. Here, this problem is solved by the hybrid FDTD-FETD method by utilizing FDTD updates in PML regions.
Figure 4.8: Normalized reflection error in $H_z$ for the hybrid FDTD-FETD and mixed-element FETD methods, for different number of PML. Reflection error levels of -54 dB and -79 dB are obtained in mixed-element FETD and hybrid FDTD-FETD methods, respectively. Hybrid method results in much lower PML reflections mainly due to the fact that FDTD exhibits twice the number of profile steps that exists in FETD.
4.5 Concluding remarks

We have described a hybrid FDTD-FETD method to simulate Maxwell’s equations in inhomogeneous and doubly-dispersive media. For the finite-element portion, a $E$-$B$ mixed vector FETD method based on first order coupled Maxwell’s equations is used. This provides convenient hybridization under leap-frog time-discretization. Due to constitutive equations that appear decoupled from the curl equations, it also produces more convenient implementation for the doubly-dispersive media, when compared to standard FETD method based on second order wave equation. A compatible pyramidal element is used to interface cubical cells of FDTD with tetrahedral elements of FETD. Accuracy and efficiency of the method is demonstrated by numerical examples. Perfectly matched layers can also be included in a straightforward fashion.
CHAPTER 5

FULL-ELECTROMAGNETIC PIC METHOD ON MULTI-GRID COMPONENTS

In this chapter, accurate and efficient plasma physics simulations in the electro- 
dynamics regime will be studied. Plasma physics aim at simulating the behavior of 
plasmas which contain large amount of free charged particles. Plasmas are involved 
in many terrestrial or extraterrestrial phenomenon such as; effect of solar wind on the 
magnetosphere, chemical reactions in the ionosphere, generation of the magnetic field 
of earth and also in plasma engines for spacecrafts [4, 5, 144–155]. Interactions of par-
ticles that make up plasma are mainly governed by electromagnetic and electrostatic 
forces. Hence analysis of plasmas require a combination of Maxwell’s equations with 
particle kinematics. In general simulations are based on three main models: particle, 
kinetic and magnetohydrodynamic models [4]. Although particle simulations offer the 
highest generality and they can most accurately capture the physics of most plasma 
problems, the latter two can produce more efficient implementations under various 
assumptions. As an example, Magnetohydrodynamics utilizes Navier-Stokes equa-
tions and assume a liquid-like behavior in the plasma [144]. Nonetheless, with the 
advment of modern computers and increasing computational power, particle models are
utilized in more and more problems. The set of equations that describe the particle model in the electrodynamic regime is given as

\[
\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \tag{5.1}
\]

\[
\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t} - \vec{J} \tag{5.2}
\]

\[
\vec{D} = \varepsilon \vec{E} \tag{5.3}
\]

\[
\vec{B} = \mu \vec{H} \tag{5.4}
\]

\[
\nabla \cdot \vec{D} = \rho \tag{5.5}
\]

\[
\nabla \cdot \vec{B} = 0 \tag{5.6}
\]

with the equations describing the particle motion and charges

\[
\frac{\partial}{\partial t} \gamma_\alpha m_\alpha \vec{v}_\alpha = q_i(\vec{E} + \vec{v}_\alpha \times \vec{B}) \tag{5.7}
\]

\[
\frac{d}{dt} \vec{u}_\alpha = \frac{\vec{v}_\alpha}{\gamma_\alpha} \tag{5.8}
\]

\[
\rho = \sum_\alpha q_\alpha \delta(\vec{u}_\alpha) \tag{5.9}
\]

Here \( \vec{E}, \vec{H}, \vec{D}, \vec{B}, \vec{u}_\alpha \) and \( \vec{v}_\alpha \) are electric and magnetic field intensity, electric and magnetic field flux density, and position and velocity of the \( \alpha \)-th particle, respectively. \( \gamma_\alpha \) is the relativistic factor and it is given by \( \gamma_\alpha = 1/\sqrt{1-(v_\alpha^2/c^2)} \). \( m_\alpha \) and \( q_\alpha \) are the mass and charge of the \( \alpha \)-th particle, respectively. \( \rho \) is the charge density and it is calculated by summing the contributions from individual particles. An important relation can be derived by taking the divergence of (5.2)

\[
\nabla \cdot \vec{J} = -\frac{\partial \rho}{\partial t} \tag{5.10}
\]
(5.10) relates the spatial change in the currents to the temporal charge in charges and is also called *continuity equation for current*.

Due to non-linearity induced by the existence of particles, solution of equations (5.1)-(5.6) in general is performed via time-domain simulation methods. In particular, FDTD and FETD solutions for the electromagnetic part of the problem have been performed. Although finite-element time-domain method offers improved modeling capabilities [156], it is not utilized in most major commercial codes due to numerical issues that have not been resolved. Furthermore, simulations based on finite-difference alone possess numerous difficulties and it is an area yet to be explored. Hence, in this dissertation we choose to focus on schemes based on the finite-difference method only.

### 5.1 Particle-In-Cell (PIC) Method

In this section a Particle-In-Cell (PIC) method based on discretization of (5.1)-(5.6) on a (staggered) Yee-cell grid with leap-frog time-integration is described. Component indices for the Yee-cell / leap-frog discretization are given as

\[
\bar{E}^n = \left( E^n_{x(i+\frac{1}{2},j,k)}, E^n_{y(i,j+\frac{1}{2},k)}, E^n_{z(i,j,k+\frac{1}{2})} \right) \tag{5.11}
\]

\[
\bar{D}^n = \left( D^n_{x(i+\frac{1}{2},j,k)}, D^n_{y(i,j+\frac{1}{2},k)}, D^n_{z(i,j,k+\frac{1}{2})} \right) \tag{5.12}
\]

\[
\bar{J}^{n+\frac{1}{2}} = \left( J^{n+\frac{1}{2}}_{x(i+\frac{1}{2},j,k)}, J^{n+\frac{1}{2}}_{y(i,j+\frac{1}{2},k)}, J^{n+\frac{1}{2}}_{z(i,j,k+\frac{1}{2})} \right) \tag{5.13}
\]

\[
\bar{H}^{n+\frac{1}{2}} = \left( H^{n+\frac{1}{2}}_{x(i,j+\frac{1}{2},k+\frac{1}{2})}, H^{n+\frac{1}{2}}_{y(i+\frac{1}{2},j,k+\frac{1}{2})}, H^{n+\frac{1}{2}}_{z(i+\frac{1}{2},j+\frac{1}{2},k)} \right) \tag{5.14}
\]

\[
\bar{B}^{n+\frac{1}{2}} = \left( B^{n+\frac{1}{2}}_{x(i,j+\frac{1}{2},k+\frac{1}{2})}, B^{n+\frac{1}{2}}_{y(i+\frac{1}{2},j,k+\frac{1}{2})}, B^{n+\frac{1}{2}}_{z(i+\frac{1}{2},j+\frac{1}{2},k)} \right) \tag{5.15}
\]

\[
\rho^n = \rho^n_{(i,j,k)} \tag{5.16}
\]
If we define the discrete version of the $\nabla$ operator based forward and backward differencing as

$$\nabla^+ \bar{f} = \left( \frac{f_{i+1,j,k} - f_{i,j,k}}{\Delta x}, \frac{f_{i,j+1,k} - f_{i,j,k}}{\Delta y}, \frac{f_{i,j,k+1} - f_{i,j,k}}{\Delta z} \right)$$

(5.17)

$$\nabla^- \bar{f} = \left( \frac{f_{i,j,k} - f_{i-1,j,k}}{\Delta x}, \frac{f_{i,j,k} - f_{i,j-1,k}}{\Delta y}, \frac{f_{i,j,k} - f_{i,j,k-1}}{\Delta z} \right)$$

(5.18)

(5.19)

discrete version of (5.1), (5.2), (5.5) and (5.6) are written as

$$\nabla^+ \times \bar{E}_n = -\bar{B}_{n+\frac{1}{2}} + \bar{B}_{n-\frac{1}{2}} \Delta t$$

(5.20)

$$\nabla^- \times \bar{H}^{n+\frac{1}{2}} = \bar{D}_{n+1} - \bar{D}_n - \bar{j}^{n+\frac{1}{2}} \Delta t$$

(5.21)

$$\nabla^- \cdot \bar{E}_n = \rho^n$$

(5.22)

$$\nabla^+ \cdot \bar{B}^{n+\frac{1}{2}} = 0$$

(5.23)

Similarly discrete version of (5.7)-(5.9) are given as

$$\frac{v_{\alpha}^{n+\frac{1}{2}} - v_{\alpha}^{n-\frac{1}{2}}}{\Delta t} = \frac{q_{\alpha}}{m_{\alpha} \gamma_{\alpha}^n} \left( \bar{E}_n + v_{\alpha}^n \times \bar{B}_n \right)$$

(5.24)

$$\frac{u_{\alpha}^{n+1} - u_{\alpha}^n}{\Delta t} = \frac{v_{\alpha}^{n+\frac{1}{2}}}{\gamma_{\alpha}^{n+\frac{1}{2}}}$$

(5.25)

$$\rho_{i,j,k}^{n+1} = \sum_{\alpha} q_{\alpha} S (\bar{X}_{i,j,k} - \bar{u}_{\alpha}^{n+1})$$

(5.26)

(5.27)

where $\bar{X}_{i,j,k}$ and $S$ are position of the $\rho_{i,j,k}^n$ in the grid and particle shape factor, respectively. A description for the particle shape factor can be found in section 5.1.3.
It is noted here that the particle position is not discretized on the Yee-grid and it is parameterized as a real-valued vector \( \vec{u}_{n+1}^\alpha \). The discrete version of the continuity equation is found by acting on (5.21) by the discrete divergence operator \( \nabla^- \) as follows

\[
\nabla^- \cdot \vec{J}^{n+\frac{1}{2}} = -\frac{\rho^{n+1} - \rho^n}{\Delta t} \tag{5.28}
\]

### 5.1.1 PIC Update Equations

By rearranging the terms in (5.20)-(5.26), update equations for the particle-in-cell method can be written as

**MAXWELL:**

\[
\tilde{H}^{n-\frac{1}{2}} = \frac{1}{\mu} \tilde{B}^{n-\frac{1}{2}} \tag{5.29}
\]

\[
\tilde{D}^n = \tilde{D}^{n-1} + \Delta t \nabla^- \times \tilde{H}^{n-\frac{1}{2}} + \Delta t \tilde{j}^{n-\frac{1}{2}} \tag{5.30}
\]

\[
\tilde{E}^n = \frac{1}{\epsilon} \tilde{D}^n \tag{5.31}
\]

\[
\tilde{B}^{n+\frac{1}{2}} = \tilde{B}^{n-\frac{1}{2}} - \Delta t \nabla^+ \times \tilde{E}^n \tag{5.32}
\]

**GATHER:**

\[
E_n^\alpha \text{ interpolation } \leftarrow E^n \tag{5.33}
\]

\[
B_{\alpha}^{n+\frac{1}{2}} \text{ interpolation } \leftarrow B^{n+\frac{1}{2}} \tag{5.34}
\]

**KINEMATICS:**

\[
\frac{v^{n+\frac{1}{2}}_\alpha - v^{n-\frac{1}{2}}_\alpha}{\Delta t} = -\frac{q_\alpha}{m_\alpha \gamma_\alpha} \left( E^n_\alpha + \frac{v^n_\alpha}{\gamma^{n+\frac{1}{2}}_\alpha} \times B^n_\alpha \right) \tag{5.35}
\]

\[
u^{n+1}_\alpha = u^n_\alpha + \Delta t \frac{v^{n+\frac{1}{2}}_\alpha}{\gamma^{n+\frac{1}{2}}_\alpha} \tag{5.36}
\]

**SCATTER:**

\[
\rho^{n+1}_{i,j,k} = \sum_\alpha q_\alpha S(\vec{X}_{i,j,k} - \vec{u}^{n+1}_\alpha) \tag{5.37}
\]

\[
\nabla^- \cdot \vec{J}^{n+\frac{1}{2}} \text{ under-constrained} = -\frac{\rho^{n+1} - \rho^n}{\Delta t} \tag{5.38}
\]
Update equations for PIC consists of four main steps: In the first step, Maxwell’s equations updates (5.29)-(5.32) are performed. This is very similar to regular FDTD updates with the addition of a specific current term $\bar{J}^{n-\frac{1}{2}}$ which has been updated in step number four of the previous iteration. This current term incorporates the effect of particles in the electrodynamic system. In the second step, an interpolation operation is performed on the updated electric and magnetic fields to obtain their values at particle locations. Since electromagnetic field components that are defined on multiple grid points are interpolated to a single point, this step is also called \textit{gather}. A more detailed explanation for this operation is given in section 5.1.4. In the third step, particle position and velocity is updated with the interpolated electric and magnetic fields. This step incorporates the particle kinematics and it is described in detail in section 5.1.2. In the fourth step, currents due to particle motion is calculated via continuity equation and additional constraints. Since multiple current components on the Yee-cell grid are updated with respect to a single particle position and velocity, this step is also called \textit{scatter}. Scatter operation is described in detail in sections 5.1.3 and 5.1.5.

### 5.1.2 Solution of kinematic equations

In general, solution of (5.35) requires substitutions

\[
\tilde{v}_\alpha^n \rightarrow (\tilde{v}_\alpha^{n+\frac{1}{2}} + \tilde{v}_\alpha^{n-\frac{1}{2}})/2 \quad (5.39)
\]

\[
\gamma^n_\alpha \rightarrow (\gamma^{n+\frac{1}{2}}_\alpha + \gamma^{n-\frac{1}{2}}_\alpha)/2 \quad (5.40)
\]

\[
\tilde{B}_\alpha^n \rightarrow (\tilde{B}_\alpha^{n+\frac{1}{2}} + \tilde{B}_\alpha^{n-\frac{1}{2}})/2 \quad (5.41)
\]
and produces an implicit equation for $\vec{v}^n$ update. Several different methods have been proposed to solve this equation; Newton, Leapfrog, Runge-Kutta and Boris-Buneman methods \cite{150,151}. Boris-Buneman method is widely used in modern PIC simulations due to its superior accuracy.

5.1.3 Particle shape factor

Particle shape factor can be thought as the distribution of a charge with respect to its origin and it is used in numerical simulations to allow interpolation of charges onto the computation grid. Particle shape factors are usually characterized with respect to their spatial width. Zeroth-order and first-order shape factors in one-dimension are written as

$$S_{1D}(u_x) = \begin{cases} 1, & \text{if } -\frac{1}{2} \leq \frac{u_x}{\Delta x} < \frac{1}{2}, \\ 0, & \text{otherwise}. \end{cases} \quad (5.42)$$

and

$$S_{1D}(u_x) = \left( 1 - \frac{|u_x|}{\Delta x} \right) \text{ if } |\frac{u_x}{\Delta x}| < 1, \quad \text{otherwise.} \quad (5.43)$$

Two and three dimensional shape factors can be calculated via $S_{2D}(u_x, u_y) = S_{1D}(u_x)S_{1D}(u_y)$ and $S_{3D}(u_x, u_y, u_z) = S_{1D}(u_x)S_{1D}(u_y)S_{1D}(u_z)$, respectively. For conservation of total charge during the movement of the particle, particle shape factor must obey the following relation

$$\sum_{i,j,k} S_{i,j,k}(\vec{u}) = 1, \forall \vec{u} \quad (5.44)$$

It is straightforward to show that the zeroth and first-order shape factors described in (5.42) and (5.43) satisfy this criterion.
5.1.4 Gather operation

In order to update the particle velocity with Lorentz force via (5.35), electric and magnetic field values at the particle positions are required. These values can be obtained by interpolating the known field values of fields components on the Yee-cell grid which are obtained via (5.29)-(5.32), to the particle location. Exact locations of the field components in Yee-cell should be taken into consideration for accurate interpolations. Linear interpolation for the fields is sufficient in most PIC algorithms.

5.1.5 Scatter operation

Calculation of the current term $\vec{J}$ in the update equation (5.21) is not straightforward since the only constraint on the current is the continuity equation that relates the divergence of the currents to the temporal change in the charges. This suggests that there exists infinite different sets of $\vec{J}$ that satisfies a given change in charge density $\rho$. A simple example demonstrating this is provided below.

Consider a 2D problem with the grid depicted in Fig. 5.1. The grid is free of charges except a point charge with associated charge density $\nabla^- \cdot \vec{D}^n = -\rho \delta_{i_c,j_c}$, that is located at the node $(i_c,j_c)$ at time-step $n$. It is moved to an adjacent node at time-step $n + 1$. The constraint on $\vec{J}$ associated with this movement can be calculated via the discrete version of the continuity equation in (5.28). It can be easily seen by inspection that both sets of current components, $\vec{J}_1$ and $\vec{J}_2$, that are shown in Fig. 5.1 produce the same change in charge density and they both satisfy (5.28). Therefore without any additional constraints they are both valid solutions. However it can also be concluded that the current density in Fig. 5.1 is more likely to be a more valid solution since it belongs to a case with a linear particle movement which
has already been introduced as an assumption in (5.24) and (5.25). The alternative solution belongs to a case with a piece-wise linear particle movement on a longer path which violates the assumptions in the kinematic equations.

It can be concluded that additional constraints are required to solve for $\bar{J}$. Several general constraints that result in simple update schemes are as follows:

1. The discrete current density $\bar{J}$ must be as similar as to the current density of a particle in the continuum with linear movement within each time-step. Although this statement only serves as a qualitative constraint, different quantitative criterion can be produced.

2. Effect of $\Delta \rho$ on $\bar{J}$ must be linear, which means if $\Delta \rho^a \rightarrow \bar{J}^a$ and $\Delta \rho^b \rightarrow \bar{J}^b$, then $\Delta \rho^a + \Delta \rho^b \rightarrow \bar{J}^a + \bar{J}^b$, where $\Delta \rho = \frac{\rho_{n+1} - \rho_n}{\Delta t}$.

3. Effect of $\Delta \rho$ on $\bar{J}$ must be space-independent, which means if $\Delta \rho_{i,j,k} \rightarrow \bar{J}_{i,j,k}$, then $\Delta \rho_{i-s,j-j_s,k-k_s} \rightarrow \bar{J}_{i-s,j-j_s,k-k_s}$, for any discrete shift $(i_s,j_s,k_s)$.

4. The above two criterion suggests a spatial stencil associated with the change in the charge density. Causality in time and space suggests that change in the charge density can not effect current components that are at distant locations and the width of the stencil must be as small as possible.

Several methodologies exist in the literature to produce algorithms that quantitatively define and satisfy the above criterion [5, 147, 148]. In the next section a brief description for the continuity-conserving scheme given in [147] will be provided.

Since spatial-changes in the currents create the temporal change in the charges, simplification on the continuity equation and expressions for the subsequent additional constraints can be obtained by rewriting the continuity equation in terms of spatial-changes instead of currents. In order to perform this operation, continuity equation
Figure 5.1: Multiple solutions can be obtained for current distribution $\bar{J}$ that satisfy the discrete continuity equation for a particular charge density, $\rho$. Therefore with discrete continuity equation per se, solution for $\bar{J}$ is under-constrained. Although not trivial, additional constraints follow from the assumptions that have been already made in discretization of the kinematics updates. In the figure circles ($\circ$) show the location of charge and charge density components, and arrows ($\uparrow$) show the location of current components. Components that are colored in black have values as indicated in the figure, and all other components are zero.
in (5.38) can be written in more explicit form as

\[- \frac{\rho^{n+1} - \rho^n}{\Delta t} = \frac{J^{n+\frac{1}{2}}_{x(i+\frac{1}{2},j,k)} - J^{n+\frac{1}{2}}_{x(i-\frac{1}{2},j,k)}}{\Delta x} + \frac{J^{n+\frac{1}{2}}_{y(i,j+\frac{1}{2},k)} - J^{n+\frac{1}{2}}_{y(i,j-\frac{1}{2},k)}}{\Delta y} \]

\[+ \frac{J^{n+\frac{1}{2}}_{z(i,j,k+\frac{1}{2})} - J^{n+\frac{1}{2}}_{z(i,j,k-\frac{1}{2})}}{\Delta z} \]  
(5.45)

Auxiliary vector \( W_{x(i,j,k)} \) is defined as

\[J^{n+\frac{1}{2}}_{x(i+\frac{1}{2},j,k)} - J^{n+\frac{1}{2}}_{x(i-\frac{1}{2},j,k)} = -q_\alpha \frac{\Delta x}{\Delta t} W_{x(i,j,k)} \]  
(5.46)

and similarly for \( W_{y(i,j,k)} \) and \( W_{z(i,j,k)} \). Substituting the \( W \) expression (5.46) and (5.37) for a single particle in (5.45) produces the first criterion on the spatial change in the currents

\[W_x + W_y + W_z = S(x^{n+1}, y^{n+1}, z^{n+1}) - S(x^n, y^n, z^n) \]  
(5.47)

where the grid indices \((i, j, k)\) are omitted for simplicity. Hypothesizing a particular form comprised of shifts of \( S(x^n, y^n, z^n) \) for \( W_x, W_y \) and \( W_z \), listing additional criterion on these functions and producing explicit formulas on \( W_x, W_y \) and \( W_z \) that satisfy all criterion along with (5.47). The recipe for \( W_x \) is reproduced below

\[W_x = \frac{1}{3} S(x^{n+1}, y^{n+1}, z^{n+1}) - \frac{1}{3} S(x^n, y^{n+1}, z^{n+1}) + \frac{1}{6} S(x^{n+1}, y^n, z^{n+1}) \]
\[- \frac{1}{6} S(x^n, y^n, z^{n+1}) + \frac{1}{6} S(x^{n+1}, y^{n+1}, z^n) - \frac{1}{6} S(x^n, y^{n+1}, z^{n+1}) \]
\[+ \frac{1}{3} S(x^{n+1}, y^n, z^n) - \frac{1}{3} S(x^n, y^n, z^n) \]  
(5.48)

Stencil associated with \( W_x, W_y \) and \( W_z \) are depicted in Fig. 5.2.

The current can be obtained by substituting (5.48) in (5.46) and solving for the current \( J_x \). The solution involves one dimensional sparse matrix equation for each problem dimension, which can be reduced to simple integration away from the boundaries for a single particle.
Figure 5.2: Auxiliary variables $W_x$, $W_y$ and $W_z$ as sums of shifted form-factors $S$. 

100
5.2 Particle-in-cell implementation in subgrids

The focus in section 5.1 has been on implementation of the PIC algorithm in single grid components with uniform cell sizes. However due to high computational cost of particle-in-cell simulations, it is usually advantageous to use multiple grid components with different cell sizes for optimization. For purely electromagnetic problems which contain no particles, subgrids have been extensively studied and numerous methods have been introduced; for examples, see [6–11, 118–122]. In PIC simulations, particles and associated fields are often localized in certain portions of the computational domain. Therefore multiple grid components can produce much higher computational savings when compared to problems purely electromagnetic in nature.

In literature there has been a specific interest on adaptive-mesh-refinement techniques, where grid component layout is dynamically adjusted for better optimization [152–155, 157]. However up to now, all of these works have been concentrated on algorithmic issues and there has been no rigorous analysis done on the performance of multi-grid methods. In electromagnetic problems, it is widely known that interfaces between different grid components are prone to numerical issues such as spurious reflections and stability problems [6]. Furthermore, spurious effects on the particle deposition operations have been observed in multi-grid PIC algorithms [157]. In this section we study issues in the continuity-conserving PIC algorithm that was described in section 5.1.5. The discussion provided here can also be generalized for other PIC algorithms that perform local deposition of currents and charges.
5.2.1 Subgridding problems in PIC

In most of the PIC algorithms current deposition is linear in a sense that currents that are deposited by two different particles do not directly interfere with each-other. Therefore, analysis of the multi-grid PIC method can be simplified by considering a single particle and its fields. In the next two sections problems that are associated with interfacing electromagnetic fields and current deposition will be discussed.

5.2.2 Problems associated with interfacing electromagnetic fields

In the multi-grid implementation, update of the field components away from the interface are trivial and performed similar to a single grid implementation. However due to change of the grid structure at the interface, a different methodology needs to be applied there. This case has been extensively studied; see [6–11, 118–122]. One major difference in the case of particles is that the electromagnetic fields may exhibit large variations at short distances due to particle static fields and motion. Therefore subgridding artifacts such as spurious reflections are expected to be much higher, and subgridding method accuracy becomes crucial. Most advanced subgridding methodologies can only produce improvements in spurious reflection levels in the order of 5-10 dB for spatial frequencies that are observed in typical PIC schemes. However recently a new subgridding method that can significantly reduce the spurious reflection levels has been introduced [6]. Subgridding by domain-overriding (SGDO) is based on extrusion of the original grid components by buffer regions composed of perfectly-matched-layers (PML), addition of smaller auxiliary grid components filled
with PML, and a set of explicit boundary operations. In this method, spurious reflection errors are eliminated, with the only major source of error being reflection from buffer PML regions. Therefore reflections can be reduced arbitrarily by controlling the number of perfectly-matched layers. A detailed description of SGDO will not be provided here. Reader may refer to [6] for a detailed explanation as well as numerical examples describing the performance of the scheme.

5.2.3 Problems associated with current deposition

Most of the popular PIC implementations perform local current depositions which deposits the currents in the vicinity of the associated particle [4, 5, 145–148], [154]. Due to this locality, interface does not directly introduce any problems in the current deposition when the particle is away from it. When the particle is in the vicinity the interface however, part of its currents remain in its home grid component, part may be at the interface, and the remaining part may be beyond the interface in the neighbor grid component. Due to the change in the grid structure at the interface and the overlapping nature of grid components, it is not straightforward how to treat these contributions. Moreover all of the available continuity conserving current deposition schemes assume single regular structured grid components, and it has not yet been generalized to multi-grid simulations. In fact, developing multi-grid schemes that conserve continuity is not trivial due to reasons that will be explained at the end of this section. Assuming that this statement true and relaxing the requirement for continuity-conservation at the interface, it is possible to produce a scheme that conserves continuity elsewhere. The required procedures are given below. Please note
here that these procedures and the remaining arguments in this section can be easily extended to local deposition schemes that are not continuity conserving.

(1) Deposit particle currents to the host grid via continuity-conserving current deposition. No decomposition is performed for any current component that is required by deposition but that is not a member of the physical portion of the grid, i.e. as a result of deposition in the vicinity of the interface. This step naturally follows from the fact that a continuity-conserving current deposition is required within each grid.

(2) Deposit particle currents to the neighbors of the host grid via continuity-conserving current deposition based on neighbor grid resolution for the currents components that are applicable. Current components that are applicable in the neighbor grid only exist when the particle is in the vicinity of the interface. This step establishes the continuity conservation at locations in the vicinity of the interface in the neighbor grids. This would otherwise be broken due to discontinuity of currents in time as the particle is transferred to the neighbor grid component.

(3) In performing the depositions in (1) and (2), make sure only one neighbor deposits on any given interface. This avoids current-doubling due to the overlapping nature of multi-grid components at the interfaces.

Given the scheme described above, continuity is guaranteed to be conserved at all node locations except the nodes at the interfaces. In order to study what would happen at the interface, let’s consider a particle traveling from a coarse grid to a fine grid as shown in Fig. 5.3. Without loss of generality, the path of the particle is chosen exactly on the boundary between cells and it is traveling normally towards the interface. At each plot grid charge at time-step $n$, $\nabla^\cdot \vec{D}^n$, and the currents at $\vec{J}^{n+\frac{1}{2}}$ are shown. At time-step $n_1$, particle charge is located at the coarse grid one cell
Figure 5.3: (a)-(d) Stuck charges that occur in an implementation where a continuity conserving algorithm is used to deposit currents onto individual grids. Stuck charge in coarse occurs since the charge is not carried further from the interface. Stuck charge with opposite sign in fine occurs since currents are withdrawn from a node that contains no charges (b). Both of these stuck charges establish static electric fields with signs that are opposite of each other. These static fields cancel out with the exception of a residue which depends on the difference in the numerical characteristic of both grids. As an example, in a case where both grids have the same resolution, static fields of these charges perfectly cancel each other without leaving any residue in electric fields.
away from the interface. Via continuity conserving deposition, the current that moves
the particle to its next location is shown in Fig. 5.3(a). At time-step \( n_2 \) the particle
charge is located at the interface and no more currents can be applied in the coarse
grid since required current component is beyond the interface outside the coarse grid.
Instead another current component is deposited in the fine grid. Since there are no
charges at the interface in the fine grid, this current components withdraws currents
from an empty location and creates a charge of opposite sign at the interface at time-
step \( n_3 \). In the same process, the original particle charge is also created. Looking
from a broader perspective, it can be noted that the total charge in the simulation
never changes in time-steps \( n_1-n_4 \). This is expected since any change in the total
charge would require an electrostatic solution. As soon as the stuck charges at the
interface are created, it can be observed that they individually emit static electric
fields with opposite signs towards both coarse and fine grids. Although the charge
pair has opposite signs, and same magnitude, they do not cancel due to the difference
in the numerical properties in coarse and fine grids. A detailed description for the
electric fields associated with the stuck charge pair is as follows.
Residual fields in regular subgridding

In a case with regular subgridding, residual static electric fields in the presence of stuck charge pair satisfy

\[
\vec{D}_c|_{i_{c+1}} = (h_D \ast \vec{D}_f|_{i_f+M_h})\downarrow M \tag{5.49}
\]

\[
\nabla^- \cdot \vec{D}_c = -\rho \delta_{i_c,j_c} \tag{5.50}
\]

\[
\nabla^+ \times \vec{E}_c = 0 \tag{5.51}
\]

\[
\vec{D}_f|_{i_f} = (h_I \ast \vec{D}_c|_{i_c})\uparrow M \tag{5.52}
\]

\[
\nabla^- \cdot \vec{D}_f = \rho \delta_{i_f,j_f} \tag{5.53}
\]

\[
\nabla^+ \times \vec{E}_f = 0 \tag{5.54}
\]

where \(D_c, D_f, E_c\) and \(E_f\) are the electric flux density and electric field intensity in coarse and fine grids respectively; \((i_c,j_c)\) and \(i_f\) are location of the stuck charge in coarse and location of the interface in fine; \(h_I\) and \(h_D\) are the filters used in interpolation and decimation and \((\uparrow M)\) and \((\downarrow M)\) are discrete interpolation and decimation operations by ratio \(M\) with \(M_h = (M + 1)/2\). Note that for the standard-subgridding method \(\nabla^- \cdot \vec{D}_n\) at any interface node is defined equal to the normal electric flux component adjacent to that node \(\nabla^- \cdot \vec{D}_n \equiv D_n\), which is equivalent to the discrete surface charge. This definition allows one to separately identify and treat the charges stuck in coarse and fine.

Residual fields in subgridding with domain-overriding

In a case with subgridding with domain-overriding, fields in either domain are equal to the sum of fields of the stuck charge in the that domain and the fields that are injected from the neighbor grid. Therefore, static electric fields in coarse grid in
the presence of stuck charge pair satisfy

\[ \nabla^- \cdot \bar{D}_c^1 = -\rho \delta_{i_c,j_c,k_c} \]  \hspace{1cm} (5.55)

\[ \nabla^+ \times \bar{E}_c^1 = 0 \]  \hspace{1cm} (5.56)

\[ \bar{D}_c^2 |_{i_c} = (h_D * \bar{D}_{f, \text{outgoing}} |_{i_f})_{i_M} \]  \hspace{1cm} (5.57)

\[ \nabla^- \cdot \bar{D}_c^2 = 0 \]  \hspace{1cm} (5.58)

\[ \nabla^+ \times \bar{E}_c^2 = 0 \]  \hspace{1cm} (5.59)

\[ \bar{D}_c = \bar{D}_c^1 + \bar{D}_c^2 \]  \hspace{1cm} (5.60)

\[ \bar{E}_c = \bar{E}_c^1 + \bar{E}_c^2 \]  \hspace{1cm} (5.61)

Here, an effective PML termination of the coarse grid for static fields is assumed at the interface in solving \( \bar{D}_c^1 \) and \( \bar{E}_c^1 \). Issues in PML termination of static fields will be discussed in the next section. The static electric fields in fine are given as

\[ \nabla^- \cdot \bar{D}_f^1 = \rho \delta_{i_f,j_f,k_f} \]  \hspace{1cm} (5.62)

\[ \nabla^+ \times \bar{E}_f^1 = 0 \]  \hspace{1cm} (5.63)

\[ \bar{D}_f^2 |_{i_f} = (h_I * \bar{D}_{c, \text{outgoing}} |_{i_c})_{i_M} \]  \hspace{1cm} (5.64)

\[ \nabla^- \cdot \bar{D}_f^2 = 0 \]  \hspace{1cm} (5.65)

\[ \nabla^+ \times \bar{E}_f^2 = 0 \]  \hspace{1cm} (5.66)

\[ \bar{D}_f = \bar{D}_f^1 + \bar{D}_f^2 \]  \hspace{1cm} (5.67)

\[ \bar{E}_f = \bar{E}_f^1 + \bar{E}_f^2 \]  \hspace{1cm} (5.68)

Again, an effective PML termination for static fields are assumed at the interface in solving \( \bar{D}_f^1 \) and \( \bar{E}_f^1 \). Note that for the SGDO method \( \nabla^- \cdot \bar{D}^n \) at any interface node is defined similar to that at the internal nodes. However only outgoing fields are used
in this calculation at the interface, so that $\nabla^{-} \cdot \hat{D}^{n} \equiv \nabla^{-} \cdot \hat{D}_{\text{outgoing}}^{n}$. This definition allows one to separately identify the charges stuck in coarse and fine.

**Removal of stuck charges**

Due to difference in numerical properties of the coarse and fine grids, electrical fields created by sum of the stuck charges exhibit a discrepancy $\hat{D}_{c} \neq 0$ and $\hat{D}_{f} \neq 0$ for both standard subgridding and SGDO method. The discrepancies are expected to be much higher than the electromagnetic fields that are created by the movement of the particles, especially in problems where speed of the particles are much lower than the speed of light $v_{p} \ll c$. Furthermore since the highest variation in the static fields of a charge is observed at small distances to the charge, the numerical discrepancy associated with the stuck charge in a coarse and fine grid are amplified at these locations. These static discrepancies remain at the interface during the simulation, accumulate as more particles travel through the interface, and exert strong non-physical forces on the particles that are passing-by. Therefore stuck charges need to be removed in order to have an accurate multi-grid PIC simulation.

In order to eliminate the stuck charges exactly, the residual electric field values $\hat{D}_{c}, \hat{E}_{c}, \hat{D}_{f}$ and $\hat{E}_{f}$ need to be calculated separately and subtracted from the total fields values in the simulation. Calculation of $\hat{D}_{c}, \hat{E}_{c}, \hat{D}_{f}$ and $\hat{E}_{f}$ in both subgridding methods require solution to an electrostatic problem similar to a Poisson solution, with the equations as described in (5.49)-(5.54), (5.55)-(5.61) and (5.62)-(5.68). Due to the fact that an implicit update is required, an exact solution to removal of stuck charges is highly computationally intensive.

An alternative method to remove the stuck charge is to use relaxation methods. These methods manipulate the divergence of the electric flux and diffuse the stuck
charges away from the interface. One important property of the relaxation methods is that they can be locally applied to a portion of the domain, when compared to Poisson solution that requires a whole-domain calculation. The only draw-back is that a local implementation for relaxation clears the residual static electric fields only in the domain of relaxation. As a result, a discontinuity at the boundary of the domain of relaxation and spurious electrodynamic waves result. Since electrostatic fields are expected to have much higher contribution in the error when compared to these electrodynamic waves, these discrepancies are usually acceptable. It is important to note here that, in a case where the domain of relaxation partially or fully includes the subgrid interface, standard subgridding may result in instabilities due to the relaxation effects that are communicated back and forth in neighbor grids. Subgridding with domain-overriding, however, does not include any feedback mechanism and is guaranteed not to introduce any immediate instability effects.

5.3 Numerical results

In this section a multi-grid implementation for the particle-in-cell (PIC) method via subgridding by domain overriding (SGDO) [6] and Marder (Langdon) relaxation [18] is studied. As described in section 5.2.1, two of the numerical problems in implementation of the PIC method on multi-grids are spurious reflections and stuck charges problems. The proposed method utilizes SGDO and Marder relaxation to reduce the former and latter problems respectively. A description for the Marder-Langdon relaxation can be found in section 5.3.3.
5.3.1 Verification: Gather

In order to test the field interpolation, a simulation with a moving charge under constant magnetic field is used. Since the force acting on the particle due to the magnetic field is perpendicular to the velocity, the particle exhibits a circular movement. Assuming negligible self-force and radiation effects [158], the equation that relates the radius of the circular path, \( r \) to the field magnitude \( B_z \), velocity magnitude \( u \) and charge \( q \) is given below

\[
r = \frac{mu}{qB_z}
\]  

(5.69)

In order to test the field interpolations, the magnetic value corresponding to a desired radius is calculated via (5.69). The projectile of the moving particle, \( u = 1 \times 10^8 \text{ m/s} \), that is obtained from the simulation is then compared to the analytical projectile. The magnetic flux value is set to \( B_z = 1.42 \times 10^{-4} \), which is expected to produce radius of 8 m. Fig. 5.4 shows that the radius of anticipated and simulated projectiles match and fields are successfully interpolated. Fig. 5.5 shows that, the velocity of the particle as it traverses the circular path is constant up to the numerical noise level in the simulation.

5.3.2 Verification: Scatter

In this section continuity conserving current deposition scheme that was described in 5.1.5 is numerically tested by considering a 2-D problem with a single particle in a grid of size 10 \( \times \) 10 cells, as shown in Fig. 5.6. In order to verify conservation of continuity: (i) \( d\rho/dt \) is numerically evaluated by using the position of the particles and (5.37) at each time step, (ii) this value is compared to divergence of the currents
Figure 5.4: Projectile of the particle under constant magnetic field. The magnitude of the magnetic field which is set to $B_z = 1.42 \times 10^{-4}$ successfully produces the anticipated radius of 8 m for the particle velocity $1 \times 10^8$ m/s.

Figure 5.5: Velocity of the particle as it traverses the circular path. It is found constant up to the numerical noise level.
obtained from the electric flux density, $\nabla^{-} \cdot \vec{J}$ in the test simulation. It can be seen from Fig. 5.6 continuity equation is successfully conserved. Fig. 5.6(e) and 5.6(e) show a slightly wider stencil for the current and the extra contribution is the non-trivial correction that is provided by the continuity conserving scheme when the particle switches cells.

### 5.3.3 Marder-Langdon relaxation convergence

A Marder-Langdon relaxation [18] diffuses the spurious discrete charges $\nabla^{-} \cdot \vec{D}$ in the electric flux density. The relaxation equations are given by

$$\vec{D}_{corr} = \vec{D} + \nabla [d_s (\nabla^{-} \cdot \vec{D} - \rho)]$$

(5.70)

with

$$\vec{D} = \epsilon \vec{E}$$

(5.71)

where $\vec{D}_{corr}$, $\vec{D}$, $\vec{E}$ are corrected electric flux density, electric flux density and electric field intensity, respectively; $\rho$ is the known discrete charge density of the particles in the PIC simulation obtained via (5.37); and $\epsilon \vec{E}$ is the permittivity including the perfectly-matched-layers (PML) tensor. Coefficient $d_s$ here is a free variable controlling the amount of correction applied. It is due to the following stability rule in 2-D

$$d_s < \frac{1}{2} \left( \frac{\Delta x^2 \Delta y^2}{\Delta x^2 + \Delta y^2} \right) = d_{max}$$

(5.72)
Figure 5.6: Conservation of continuity is verified by comparing the $\nabla^+ \cdot \vec{J}$ value obtained from the simulation with the charge density separately obtained by evaluating Eq. (5.37) separately. (e) and (f) shows a wider stencil for the current where the extra component is due to the non-trivial compensation into the old cell as the particle switches cells.
In the following section a numerical convergence analysis of the Marder-Langdon scheme with respect to parameter $d_s$ is presented. A domain composed of a single grid with size $21 \times 21$ cells and cell-size $1 \times 1 \text{m}^2$ is used. A charged particle is placed at the center of the domain at $(x_p, y_p) = (10.5, 10.5)$ with an associated charge distribution $\rho$. The electric fields are initialized to zero with $\nabla \cdot D = 0$ and they are corrected by 1,000 iterations of Marder-Langdon correction. In order to obtain the reference field distribution, results of 10,000 iterations of Marder-Langdon correction is used. Error in this reference solution is estimated to be in the order of $-200 \text{dB}$. The error is calculated by using the spatial average of the errors and normalizing it by the maximum of $\rho$, as

$$\frac{\sum_{i,j} (\nabla - \cdot \bar{D} - \rho)}{N_i N_j \max (\rho)}$$

(5.73)

Fig. 5.7 shows the convergence of the Marder-Langdon scheme with respect to parameter $d = d_s/d_{\text{max}}$. A logarithmic decrease in the error is observed with respect to time-step, where higher convergence rates are observed for higher $d$. A convergence rate of 10 dB per 105 iterations is observed for $d = 1$. We would like to stress here that an important factor in convergence is the spectral frequency spectrum of $\rho$. In particular, charge distributions without significant low-frequency components tends to require much less iterations to converge. A point charge, as in our example, has equal spectral contribution in all frequencies and it therefore requires as much as 550 iterations for a -60 dB improvement. A detailed study on the performance of the method with respect to spectral frequency can be found in [18].

It was observed in 5.7 that a high number of iterations required to reduce the error in the Gauss-law for a single particle. However in practical situations with
Figure 5.7: Normalized average spatial error with respect to number of iterations for different values of the correction coefficient $d = d_s/d_{max}$. Higher convergence is observed for higher $d$ values. A convergence rate of 10 dB per 105 iterations is observed for $d = 1$. 
high number of charges, the low frequency components of the total charge that is accumulated along the interface is much smaller due to averaging effects. Hence much higher convergence rates are expected.

5.3.4 Verification: Accuracy

The accuracy of the method is studied by comparing three different Marder-Langdon correction implementations; full-domain, towards-PML only, and interface-only, with reference coarse and fine single grid solutions. A domain with size \(21 \times 21\) cells with coarse cell-size \(1 \times 1\) m\(^2\) is used. Two particles with opposite signs are initially placed at \((x_{e,p}, y_{e,p}) = (12.6, 4.2)\), with one moving with velocity \(v_e = (-0.23, 0.76, 0)\)c, where \(c\) is the speed of light, and the other one with zero velocity, \(v_p = (0, 0, 0)\). The interface is located \(y = 11\) m. A refinement ratio of 3 is used in cases with refinement. An all-coarse, an all-fine case and a case without correction is used as reference. Marder correction is applied at each time-step iteratively until the residual spurious charge density \(\nabla^- \cdot \bar{D} - \rho\) is lower than \(1 \times 10^{-3}\)th of the charge density associated with a single particle. In the Marder relaxation implementation towards PML, correction is applied at all domains in the SGDO buffer region including the interface. In calculation of \(\nabla^- \cdot \bar{D}\) at the interface, only outgoing fields are used in consistence with section 5.2.3. The electric field is observed at 108’th time-step after the particle passes through the interface, and it is interpolated to node-locations for the wave field plot. A Courant factor of \(CN = 0.98\) is used.

It can be observed from Fig. 5.8 that, spurious fields are observed in no-correction, full-domain and interface-only simulations, where the strongest discrepancies exist in the interface-only simulation. Part of the all-coarse field values are found unresolved.
Figure 5.8: Electric fields at time step $T_{\text{max}} = 108$ for different scenarios. Spurious fields are observed in no-correction, full-domain and interface-only simulations. All-coarse field values are unresolved. toward-PML implementation can successfully simulate this problem.
Toward-PML implementation produced the least discrepancy when compared to other alternatives.

### 5.3.5 Laser-foil interaction

Figure 5.9 compares the electric field and electron energy for a 1D laser-plasma interaction problem. Fine grid is located on the left-hand side with size 600 fine cells, whereas the coarse region is located on the right-hand side with size 200 coarse cells. A refinement ratio of 2 is used in the fine region. Initially, 20 particles per cell is used in coarse and fine with a Maxwellian velocity distribution [144]. A sine modulated Gaussian pulse is used as the excitation. Courant number [1] is chosen as $C_N = 0.5$. Two additional simulations with all-coarse and all-fine grids are used as references. Each row of the plot is associated with a different case, which can be listed top to bottom as; a uniform fine simulation as reference, SGDO, contour-integration, mixed-integration and a uniform-coarse simulation.

Fig. 5.9 shows the electric fields and the electron energy snapshots taken when two-thirds of modulated Gaussian pulse advanced through the interface. It can be seen in the longitudinal wake field $E_x$ plots that significant disturbances are observed in the proximity of the fine-coarse interface, in the case of contour and mixed integrations. The effect of disturbance is also observed in the plot of electron energy. In the all-coarse case, disturbances due to unresolved fields are observed. On the other hand, all-fine and subgridding with domain overriding cases match only with minor discrepancies. It can be concluded that subgridding with domain-overriding can significantly improve the accuracy in subgrid plasma simulations.
Figure 5.9: Electric field and electron energy for the 1D laser-plasma interaction problem. Fine and coarse grid interface is indicated in the figure as the dotted line. Subgridding with domain-overriding shows significant improvements when compared to other methods. Significant artifacts are observed at the interface for contour- and mixed-integration.
5.4 Concluding remarks

Efficient implementation of full Electromagnetic particle-in-cell (PIC) algorithm on multiple grid components is described. The algorithm is based on updates similar to that in FDTD with the addition of particle kinematic equations that describe the movement of the particles. Although single-grid implementation of the PIC algorithm produces accurate results, multi-grid implementation is plagued with two significant numerical problems that are associated with the interface; (i) spurious reflections due to interfacing of the electromagnetic fields, (ii) static electric fields due to stuck charges that are created due to continuity conservation that breaks down at the interface. These problems not only pollute Electromagnetic fields, but also result in spurious forces on the particles and can significantly affect the accuracy. In order to alleviate (i), a subgridding by domain-overriding (SGDO) algorithm is employed. In order to alleviate (ii), an efficient Marder relaxation technique is used. Marder relaxation is locally applied on the non-physical regions associated with SGDO and can effectively remove stuck charges with the expense of a smaller electromagnetic disturbance. Accuracy of the method is demonstrated by quantitative and qualitative numerical tests.
CHAPTER 6

CONCLUSIONS

In this dissertation, improved time-domain simulation methods for electrodynamics and plasma physics problems has been studied. In particular, the focus has been on two of the most popular time-domain simulation methods, finite-element time-domain (FETD) and finite-difference time-domain (FDTD).

A $E-B$ mixed vector FETD method based on discretization of Maxwell’s first order coupled equations is studied. This method utilizes a combination of electric field and magnetic flux as state variables and produces update equations similar to those in FDTD under leapfrog discretization. The only significant difference is that update equations in FETD includes sparse matrices and requires an implicit sparse matrix solution. $E-B$ FETD method utilizes compatible Hodge (mass) matrix definitions based on differential forms, and it exhibits several advantages when compared to the regular FETD method based on the second order wave equation. Two of these advantages are: (i) easier implementation for doubly-dispersive media, and (ii) easier hybridization with FDTD.

Exploiting item (i), $E-B$ mixed vector FETD method is extended to doubly-dispersive media, which exhibits frequency-dispersion simultaneously in permittivity and permeability. In particular, a general material profile consisting of ratio of two
polynomials on frequency is used. This profile can recover most of the popular dispersive models, such as: Debye, Lorentz and Drude models. A cell-based discretization is used for the material distribution which results in desirable symmetrical Hodge matrices. Constitutive relations for the doubly-dispersive case are simplified by separating individual contributions from different axis directions and different cells. This produces a simple, FDTD-like dispersion implementation except for the fact that more terms are required. It has been demonstrated by numerical examples that the proposed method can accurately simulate doubly-dispersive materials.

Perfectly-matched layers (PML) is an absorbing boundary condition that is used to simulate open-domain problems. Due to the fact that it can be represented as an effective doubly-dispersive material distribution, $E$-$B$ FETD method can provide straightforward and consistent PML implementations. In this dissertation, rectangular and conformal implementations have been considered. It has been demonstrated by numerical examples that satisfactory reflection levels can be obtained in both implementations. However, it has been also shown that implementations of perfectly-matched layers in FETD based on cell-based material definitions exhibit slower convergence of reflection error with respect to number of layers, when compared to that in FDTD. This has been attributed to the fact that FDTD assigns two material profile points per each cell, whereas FETD assigns only one. It has been further shown that optimal value of maximum conductivity is half of that in FDTD.

Exploiting item (ii), $E$-$B$ mixed vector FETD method is further hybridized with FDTD. Due to the fact that the latter can be expressed as an approximation to the former, these methods constitute a good choice for hybridization. Furthermore, both methods utilize the same time-integration methodology, ie. leapfrog, and no
interfacing in time is required for hybridization. The geometrical interfacing however, is not straightforward since tetrahedral cells of FETD and octahedral cells of FDTD can not be directly connected. In order to establish the transition, a compatible pyramidal element based on differential forms discipline has been utilized. It has been shown via numerical examples that the proposed method can accurately simulate doubly-dispersive materials.

Full-electromagnetic particle-in-cell (PIC) method is widely used in plasma physics and provide accurate simulations of plasma phenomenon. In this method, the electromagnetic portion of the problem is discretized on a Yee-grid with leapfrog time-integration. Therefore it exhibits update equations akin to that in FDTD. On the other hand, modeling of the particles are realized by quasi-particles that are macroscopic descriptions of physical particles based on real valued (non-discretized) position and velocity variables. The particles interact with FDTD through current terms, whereas electric and magnetic fields in FDTD interact with particles through the Newton-Lorentz relation that is used in the kinematic updates that govern the movement of the particles. In this dissertation, a full-electromagnetic Particle-in-cell (PIC) implementation on multiple grid components is introduced. Similar to problems purely electromagnetic in nature on subgrids, multi-grid PIC implementations are also plagued by numerical artifacts that are; spurious reflections and static fields due to stuck charges at the interface. In order to alleviate the spurious reflections problem, subgridding by domain-overriding (SGDO) method is introduced. Removal of stuck charges are performed by a local and efficient Marder relaxation which takes advantage of the SGDO buffer regions. The proposed algorithm can significantly reduce the numerical artifacts listed above.
APPENDIX A

CONSTANTS USED IN SOLVING DISPERSIVE RELATION

The constants $w_x(k_{1i})$, $u_x^{(p)}(k_{1i})$ and $v_x^{(p)}(k_{1i})$ in (2.26)-(2.27) are given in terms of material parameters $q_x(k_{1i})$ and $r_x^{(p)}(k_{1i})$ below for a general dispersive model with $N_p = 4$. Since the face index is the same throughout all equations below, it is omitted for simplicity. Expressions for $w_y(k_{1i})$, $u_y^{(p)}(k_{1i})$ and $v_y^{(p)}(k_{1i})$ can be obtained by simply replacing $x$ by $y$ below.
\[ u_x^{(0)} = \Lambda_x^{-1}(\tau q_x^{(0)} + \tau^2 q_x^{(2)} + \tau^3 q_x^{(3)} + \tau^4 q_x^{(4)}) \]  
\[ u_x^{(1)} = \Lambda_x^{-1}(q_x^{(1)} + 2\tau q_x^{(2)} + 2\tau^2 q_x^{(3)} + 2\tau^3 q_x^{(4)}) \]  
\[ u_x^{(2)} = \Lambda_x^{-1}(q_x^{(2)} + 2\tau q_x^{(3)} + 2\tau^2 q_x^{(4)}) \]  
\[ u_x^{(3)} = \Lambda_x^{-1}(q_x^{(3)} + 2\tau q_x^{(4)}) \]  
\[ u_x^{(4)} = \Lambda_x^{-1} q_x^{(4)} \]  
\[ w_x = \Lambda_x^{-1}(r_x^{(0)} + \tau r_x^{(1)} + \tau^2 r_x^{(2)}) \]  
\[ + \tau^3 r_x^{(3)} + \tau^4 r_x^{(4)} \]  
\[ \]  
\[ v_x^{(0)} = \Lambda_x^{-1}(\tau r_x^{(1)} + \tau^2 r_x^{(2)} + \tau^3 r_x^{(3)} + \tau^4 r_x^{(4)}) \]  
\[ v_x^{(1)} = \Lambda_x^{-1}(r_x^{(1)} + 2\tau r_x^{(2)} + 2\tau^2 r_x^{(3)} + 2\tau^3 r_x^{(4)}) \]  
\[ v_x^{(2)} = \Lambda_x^{-1}(r_x^{(2)} + 2\tau r_x^{(3)} + 2\tau^2 r_x^{(4)}) \]  
\[ v_x^{(3)} = \Lambda_x^{-1}(r_x^{(3)} + 2\tau r_x^{(4)}) \]  
\[ v_x^{(4)} = \Lambda_x^{-1} r_x^{(4)} \]  

where

\[ \Lambda_x = q_x^{(0)} + \tau q_x^{(1)} + \tau^2 q_x^{(2)} + \tau^3 q_x^{(3)} + \tau^4 q_x^{(4)} \]  
\[ \tau = 2\Delta t^{-1} \]
Subgridding with domain-overriding (SG-DO) algorithms require a large number of buffer and auxiliary sub-domains based on the problem dimensions and number of interfaces. Fig. B.1(a) shows the simplest implementation of the SGDO algorithm. In this case both fine and coarse grids are extruded by perfectly-matched layers and two additional sub-domains are used.

A two-dimensional split is realized by systematic subgridding of all four individual grids shown in Eq. (B.1). This operation requires extrusion of the grids at the new interface and addition of respective auxiliary grids (two per each grid). A similar treatment is given to the update equations at the interface for SGDO, where existing update equations are superposed with new equation sets that are obtained for each new subgridding interface. In the two dimensional split described, a total of 16 grids are required. Fig. B.2 shows the associated grid formation. Further calculations indicate that a three-dimensional split would require 64 grids, each with its respective update equations.

In summary, due to high number of grids involving the SGDO implementation, hard-coding for certain grid types is highly impractical and a systematic approach needs to be followed. For SGDO, it is possible to formulate an algorithm that splits
Figure B.1: (a) shows the grid layout in a 3D subgridding with domain-overriding problem. Individual grids are highlighted in (b), (c), (d) and (e). The conductivity scaling of PML is also illustrated in the figures.
the domain and generates a table that contains the grid geometry and connectivity information. The algorithm for such implementation is given below. It is important to note here that, although the algorithm provided here is not recursive, it results in recursive division of grids as it progresses.

01. Loop over all split planes $P_i$, each of which is perpendicular to an axis

02. Loop over all grids $\Omega_j$

03. Skip to next grid if $P_i \cap \Omega_j = \emptyset$

04. Split $\Omega_j$ by $P_i$ into two pieces: $\zeta_1$, $\zeta_2$

05. Extrude each piece $\zeta_q$ by the desired PML length $N_{PML}$ at the interface

06. Add two new auxiliary domains $\Omega_1$, $\Omega_2$ to the $\Omega$ list

07. Modify PML lengths in $\zeta_1$, $\zeta_2$, $\Omega_1$, $\Omega_2$ that are normal to the interface
08. Add new modified SGDO update equation region $\Xi_1$

09. Split all $\Xi_q$ that intersect $P_i$

10. End grid loop

11. End split plane loop

Fig. B.1 shows the result of the recursive SGDO grid-generation algorithm for a $2 \times 2$ split in 2D. The grids are ordered with respect to the number of auxiliary levels that has been travelled: Four square shaped grids at the bottom (note that only two of them are visible) are physical grids which would also exist in a standard subgridding algorithm. The higher level highly skewed rectangular grids are auxiliary domains associated with the physical grids at the lower level. Finally, four small square grids on top are second order auxiliary domains that connect the first order auxiliary grids. In a 2D case, there can be at most two levels, whereas in 3D three levels are possible.

Fig. B.3 also shows the field snapshot for a line source excitation problem in free space. The source is located at the small white dot at the bottom of Fig. B.3 and it is driven by an ultra-wide-band source excitation. Bottom tile is assigned as a fine grid, whereas all the other three physical grids are coarse. It can be seen from this qualitative test that no spurious reflections are visible at the subgrid interfaces and exterior PML layers. It can be concluded that the recursive SGDO grid generation is successfully implemented up to the visible reflection level.

In order to verify the qualitative results, normalized residual errors are calculated in a setup with a one-dimensional split. The subgrid interface is placed at $x_i = 20$ m in a computational domain with size $40 \times 50$ m$^2$. Source and probe are located
Figure B.3: SGDO subgrids created by the recursive grid generation algorithm for a 2D case for a $2 \times 2$ tile of Fig. B.2. All grid tiles except the bottom tile are coarse domains. A magnetic field snapshot is placed on top of the grids. Location of the line-source can be seen in the lower corner as a white point. An ultra-wide-band Blackmann-Harris pulse source excitation is used. The physical domains are seen as large square regions at the bottom of the grid stack, whereas the smaller auxiliary SGDO regions are on higher stacks.
at \((x_s, y_s, z_s) = (5, 25, 2.5)\) m and \((x_p, y_p, z_p) = (15, 25, 2.5)\), respectively. A derivate
Gaussian excitation is used for the source with the driving function

\[
M_z(x_s, y_s, z_s) = (T/2 - t) \exp^{-32 \left(\frac{t-T/2}{T}\right)^2}
\]  

(B.1)

where \(T = 180\Delta t\) is the period of the source excitation and \(\Delta t\) is the time-step. A
refinement ratio of 3 is used in all directions. An all-fine grid is used as the reference.

The error is calculated as

\[
Err^{(n)}(i_p, j_p) = 20 \log_{10} \left( \frac{H_{zsg}^{(n)}(i_p, j_p) - H_{zref}^{(n)}(i_p, j_p)}{\max_n(H_{zref}^{(n)}(i_p, j_p))} \right)
\]  

(B.2)

The normalized error is shown in Fig. B.4.

Figure B.4: Normalized residual error at the probe location for the half-space problem.
It can be observed from Fig. B.4 that SGDO produces approximately -35 dB lower spurious reflection levels when compared to the standard subgridding scheme with constant filters. These levels are consistent with that reported in [6].
BIBLIOGRAPHY


