HIGH ORDER FDTD METHODS FOR ELECTROMAGNETIC SYSTEMS
IN DISPERSIVE INHOMOGENEOUS MEDIA

by
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ABSTRACT

This dissertation presents matched interface and boundary time-domain (MIBTD) methods for solving both transverse magnetic (TM) and transverse electric (TE) Maxwell’s equations in non-dispersive and dispersive media with complex interfaces and discontinuous wave solutions. In this thesis, five following problems will be discussed: (1) Dielectric interface problems; (2) Debye dispersive interface problems in TM mode; (3) Drude dispersive interface problems in TM mode; (4) Debye dispersive interface problems in TE mode; and (5) Perfectly matched layer (PML) boundary conditions for dispersive interface problems. It is well known in the electromagnetic interface problems that field components across the interfaces are often nonsmooth or even discontinuous. Consequently, the finite-difference time-domain (FDTD) algorithms without a proper interface treatment will cause a staircasing error when dealing with arbitrary interfaces; and only first-order of accuracy is achieved by those FDTD methods. Thus, to restore the accuracy reduction of the collocation FDTD approach near an interface, the physical jump conditions relating discontinuous wave solutions on both sides of the interface must be rigorously enforced. For this purpose, a novel matched interface and boundary (MIB) scheme is proposed to handle material interface problems, in which new jump conditions are derived so that the discontinuous and staggered features of electric and magnetic field components can be accommodated. That results in the staircasing error is totally eliminated in the dielectric interface problems. However, in the dispersive materials like Debye media, interface conditions are now time-dependent. Thus, interface auxiliary differential equations (IADEs) are utilized to describe the transient changes in the regularities of electromagnetic fields across a Debye dispersive interface. In addition, in TM mode, to assist the track of the jump condition information along the interface, a novel hybrid system, which couples the wave equation for the electric component with Maxwell’s equations for
the magnetic components, is constructed based on the auxiliary differential equation (ADE) approach. As a result, the staircasing error is also eradicated for the Debye interface problems. However, this MIBTD approach is only designed for Debye material equations formed by first-order ADE. Because of that, the MIBTD algorithm for the problem (2) cannot be directly extended to solve Drude dispersive interface problems having second-order ADE. To achieve high order accuracy for the problem (3), a novel hybrid Drude-Maxwell system and IADEs are also formulated to update the regularity change of the field components across interfaces so that the staircasing error is free in the numerical results. In the dispersive interface problems in TE mode, the jump conditions of the electric components become more complicated than in the TM mode case, and rigorously depend on the unknown flux density fields. Therefore, the standard Maxwell’s equations are taken into consideration instead of the hybrid system. The leapfrog scheme is employed to simplify the complexities of the jump conditions’ derivations in the TE mode, whereas the fourth-order Runge-Kutta method is exploited in the other cases. In any material interface problems, effective MIB treatments are proposed to rigorously impose the physical jump conditions which are not only time dependent, but also couple both Cartesian directions and different field components. Based on a staggered Yee lattice, the proposed MIB schemes can achieve up to sixth order-accuracy in dealing with the straight interfaces, while the uniform second-order accuracy is always maintained in solving irregular interfaces with constant curvatures, general curvatures, and nonsmooth corners. Based on the numerical verification, our MIBTD algorithms are conditionally stable and more cost-efficient than the classical FDTD methods. Finally, the Berenger’s PML is successfully used as absorbing boundary condition (ABC) for the dispersive interface problems. The numerical results are provided to validate the efficiency of that PML ABC.
DEDICATION

I dedicate this dissertation to my parents Loc Nguyen and Hong Tran.

To my wife Hoa Bui and my son Andrew Nguyen.

To my brothers and sisters.
LIST OF ABBREVIATIONS AND SYMBOLS

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>TM</td>
<td>Transverse-magnetic mode</td>
</tr>
<tr>
<td>TE</td>
<td>Transverse-electric mode</td>
</tr>
<tr>
<td>TEM</td>
<td>Transverse electromagnetic</td>
</tr>
<tr>
<td>ADE</td>
<td>Auxiliary differential equation</td>
</tr>
<tr>
<td>PLRC</td>
<td>Piecewise-linear recursive-convolution</td>
</tr>
<tr>
<td>ODE</td>
<td>Ordinary differential equation</td>
</tr>
<tr>
<td>PDE</td>
<td>Partial differential equation</td>
</tr>
<tr>
<td>RK4</td>
<td>Fourth-order Runge-Kutta method</td>
</tr>
<tr>
<td>FDTD</td>
<td>Finite-difference time-domain</td>
</tr>
<tr>
<td>CFL</td>
<td>Courant-Friedrichs-Lewy</td>
</tr>
<tr>
<td>PEC</td>
<td>Perfect electric conductor</td>
</tr>
<tr>
<td>PML</td>
<td>Perfectly matched layer</td>
</tr>
<tr>
<td>BPML</td>
<td>Berenger's PML</td>
</tr>
<tr>
<td>CPML</td>
<td>Convolution PML</td>
</tr>
<tr>
<td>CEM</td>
<td>Computational electromagnetics</td>
</tr>
<tr>
<td>MIB</td>
<td>Matched interface and boundary</td>
</tr>
<tr>
<td>MIBTD</td>
<td>MIB time-domain</td>
</tr>
<tr>
<td>MIBTD2</td>
<td>Second-order MIBTD</td>
</tr>
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</table>
MIBTD4  Forth-order MIBTD
MIBTD6  Sixth-order MIBTD
IADE   Interface auxiliary differential equation
E     Electric field
D     Electric flux density
H     Magnetic field
B     Magnetic flux density
ε     Permittivity
μ     Permeability
ε₀    Free-space permittivity
μ₀    Free-space permeability
εᵣ    Relative permittivity
μᵣ    Relative permeability
qₑs   Surface electric charge density
Jₛ    Induced linear electric current density
^     Phasor quantity
ω     Angular frequency
εₛ,p, εₛ    Permittivity at static frequency
εₘ     Permittivity at high frequency limit
j     Imaginary unit
γ, γₚ    Relaxation time constant
ωₚ, ω₁    Frequency of the pole pair
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$\sigma_p$</td>
<td>Damping coefficient.</td>
</tr>
<tr>
<td>$\Delta x$</td>
<td>Lattice space increment in the $x$ direction</td>
</tr>
<tr>
<td>$\Delta y$</td>
<td>Lattice space increment in the $y$ direction</td>
</tr>
<tr>
<td>$\Delta t$</td>
<td>Time increment</td>
</tr>
<tr>
<td>$\vec{n}$</td>
<td>Normal vector</td>
</tr>
<tr>
<td>$\vec{\tau}$</td>
<td>Tangential vector</td>
</tr>
<tr>
<td>$\mathbb{C}$</td>
<td>Complex number set</td>
</tr>
<tr>
<td>$\ast$</td>
<td>Convolution</td>
</tr>
<tr>
<td>$\mathcal{F}^{-1}$</td>
<td>Inverse Fourier transform</td>
</tr>
</tbody>
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Chapter 1

INTRODUCTION

Dispersive medium, in which the permittivity is a function of frequency [1–3], is often encountered in nature, such as in biological tissues, rocks, soils, ice, snow, and plasma. Due to such a omnipresent nature, the study of dispersive materials is indispensable to a wide range of electromagnetic applications. For instance, the ground penetrating radar (GPR) is a widely used nondestructive testing tool for subsurface sensing and detection of buried objects [4]. At the operating frequency range of the GPR, soil materials are known to exhibit strong frequency dispersion. Recently, microwave imaging has emerged as a promising alternative to the X-ray mammography for the early detection of breast cancer [5]. Similarly, the breast tissues are quite dispersive over the frequency band of interest in the microwave breast imaging. In these electromagnetic applications, to validate the experimental designs, the modeling of material dispersiveness is important for studying electromagnetic wave scattering and propagation in dispersive media. Moreover, in both the GPR and microwave breast imaging, there is usually a significant contrast in the dielectric properties between the target, such as mines or malignant tumors, and its surrounding. In practice, there is a pressing need to develop robust numerical tools to simulate how an electromagnetic wave interacts with a dispersive interface [6–10], which is defined to be the material boundary between a dispersive medium and a non-dispersive medium or between two dispersive media.

It is well known in the CEM literature that across material interfaces, field components are nonsmooth or even discontinuous [25, 26]. The dispersive finite-difference time-domain (FDTD) methods without proper interface treatment will produce a staircasing error in
dealing with arbitrary interfaces [1, 18–21]. The accuracy reduction of the staircasing approximation can be partially recovered by using smoothing techniques [22–24], in which the permittivities in the vicinity of an interface are averaged to form a smooth effective permittivity. However, those approaches still cannot attain the second-order accuracy. By using unstructured grids or adaptive grids, the dispersive finite element time domain-methods (FETD) [11–14] and dispersive discontinuous Galerkin time-domain (DGTD) methods [15–17] are some of the most flexible methods for handling geometrically complex problems in the numerical solution of Maxwell’s equations over dispersive media. Nevertheless, those approaches require mesh generation for each interface problem. Therefore, there is a need to develop high order FDTD methods.

In the high order FDTD approaches, special interface treatments in which the interface conditions are properly imposed in the discretization, are indispensable. For nondispersive interfaces, many such high order interface treatments have been developed in the literature [25, 27–33]. However, the generalization of such rigorous interface treatments to dispersive interfaces is extremely challenging, because a new difficulty is encountered in a dispersive interface problem. In particular, the wave solution will lose its regularity in a time variant manner across a dispersive interface [6–10]. In other words, the jump conditions at a dispersive interface are time dependent, whereas their counterparts for a nondispersive interface are time independent. The rigorous interface treatment for imposing time variant jump conditions is less well developed in the literature.

Recently, novel dispersive FDTD algorithms based on the matched interface and boundary (MIB) method [26, 34] have been developed for solving one-dimensional (1D) transverse electromagnetic systems [6]. An auxiliary differential equation (ADE) approach is employed in these dispersive FDTD methods [6] to model the constitutive conditions. Moreover, the unsteady jump conditions are also reformulated by using the ADE approach into a form that can be rigorously incorporated in the FDTD discretization. High order convergences are numerically confirmed in solving 1D Maxwell’s equations. However, the previous dispersive
MIB approaches [6] can only handle one-dimensional case and continuous solutions.

The generalization of the dispersive MIB methods to accommodate higher dimensional case, arbitrarily curved interfaces and discontinuous solutions is of practical importance, and is the main objective of this dissertation. At first, we developed a new MIB time-domain (MIBTD) method for solving 2D TM and TE Maxwell’s equations with curved dielectric interfaces based on a simple Cartesian grid. In this MIBTD method, a novel formulation of jump conditions will be proposed, so that the discontinuous and staggered features of electric and magnetic field components can be accommodated. This facilitates the implementation of the jump conditions in the FDTD discretization and suppresses the staircase approximation errors completely over the Yee lattices. The present study represents a considerable progress on the development of MIBTD methods for solving Maxwell’s equations, because the proposed MIBTD method is the first of its kind that can handle discontinuous electromagnetic waves. This result is reported in our published work [54], and discussed in Chapter 3.

However, the method presented in [54] only handle the non-dipsersive interface problems. Specifically, that MIBTD method is proposed to deal with the time-independent jump conditions. In Dispersive medium, the interface conditions are known to be time-dependent. In our work [7, 8], based on the ADE approach, the Debye dispersion model is coupled with the TM equations to derive interface auxiliary differential equations (IADEs) for describing the regularity changes in electromagnetic fields at dispersive interfaces. Also, a novel hybrid Debye-Maxwell system is formulated so that one can easily track the transient changes of the field components along the interfaces. The enforcement of the resulting time dependent jump conditions fits the finite difference weights to the dispersive interfaces, so that the staircasing error is eliminated. A uniformly second order of accuracy can be achieved in solving various dispersive interfaces. Chapter 4 reports this result.

Though the MIBTD algorithms presented in Chapter 4 successfully handle the loss in waves’ regularities, but only Debye model is investigated. Another dispersive medium like Drude model still cause some issues. In particular, the auxiliary differential equation (ADE)
of the Drude material is a second order differential equation while that of the Debye medium is just first order (see Eqs. (2.3.4) and (2.3.7)). It can be argued that the Drude model may be decomposed into a linear combination of a Debye model and a constant-conductivity model; consequently, only first order ADEs like the Debye material case are involved. Unfortunately, this approach requires the jump conditions for the current density which yield numerous impediments in carrying out the MIBTD algorithm. Therefore, the second-order ADE described in Eq. (2.3.7) is more manageable for the MIBTD modeling. Similar to the Debye interface problems, a novel Drude-Maxwell system, which gives rise to the wave equation coupling the electric and magnetic components of the Maxwell’s equations, is also formulated. This algorithm is discussed in our paper [9], and presented again in Chapter 5.

In the previous MIBTD methods which will be reported in Chapters 4 and 5, only TM mode is considered. These MIBTD methods cannot be directly generalized to solve transverse electric (TE) Maxwell’s equations, which now have discontinuous wave solutions across the dispersive interface. Mathematically, the essential challenge of the MIBTD formulation for TE systems is due to the complexity in the interface conditions for the electric components \( \mathbf{E} = (E_x, E_y, E_z) \). For the TM mode, we have simply one zeroth order jump condition saying that \( E_z \) is continuous [6–8], whereas we need two zeroth order jump conditions for \( E_x \) and \( E_y \) in the TE mode. Moreover, the conditions for \( E_x \) and \( E_y \) are time dependent and are coupled with the unknown electric flux density components \( D_x \) and \( D_y \). Therefore, the construction of new jump conditions within a proper Maxwell formulation is indispensable for developing embedded FDTD methods for solving TE type dispersive interface problems. Unlike our TM studies [6–9], we will not use the hybrid Maxwell governing equations. Instead, the standard TE Maxwell’s equations will be adopted, because they turn out to be better for the modeling of the TE jump conditions. Based on the ADE approach, the Debye dispersion model is coupled with the TE equations to derive interface auxiliary different equations (IADEs) for describing the regularity changes in the electromagnetic fields at dispersive interfaces. Comparing with the TM cases, we find that there are more IADEs in the present
TE study and their numerical implementation becomes more involved, but is still feasible using the MIB scheme. Because the standard Maxwell’s equations are employed for the present TE problem, the leapfrog scheme can be simply utilized for time integration. This is more efficient than the fourth order Runge-Kutta scheme in our previous TM works [6–9] for solving the hybrid Maxwell’s equations. With these theoretical and numerical developments, the proposed MIBTD method achieves a uniformly second order of accuracy in solving various TE dispersive interface problems. To the best of our knowledge, the proposed MIBTD method is the first high order embedded FDTD method developed in the CEM literature for solving TE Maxwell’s equations with inhomogeneous dispersive media.

By the motivation of simulating the dispersive interface problems in a long time, an effective absorbing boundary condition (ABC) is taken into account. In 1994, Berenger published a paper [51] to propose a new ABC named perfectly matched layer (PML). In this thesis, we successfully integrate the Berenger’s PML (BPML) into our interested interface problems. The numerical results indicates that our proposed methods for material interface problems are still stable at a long-time simulation.

The rest of the dissertation is organized as follows. Chapter 2 will discuss general Maxwell’s equations. The ADE expressions for different dispersive media is provided. Also, the classical finite-different time-domain method, i.e Yee scheme, is presented to discretize TM and TE modes. Finally, this chapter ends with a discussion of boundary condition and absorbing boundary layer. In Chapter 3, proposed MIBTD algorithms for solving the dielectric interface problems is offered. Chapter 4 is devoted for the MIBTD methods for Debye dispersive interface problems in the TM mode. That kind of methods designed for the Drude dispersive interface problems in the same mode is introduced in Chapter 5. We will present the novel MIBTD schemes for Debye dispersive interface problems in TE mode in Chapter 6. The simulations of the previous dispersive interface problems with the use of BPML are provided in Chapter 7. Finally, a conclusion ends this dissertation.
Chapter 2

ELECTROMAGNETIC THEORY

2.1 Maxwell’s equations

In this section, we consider the general forms of Maxwell’s equations in three dimensions. The simplified two-dimensional cases then, are conducted.

2.1.1 Maxwell’s equations in three dimensions

Maxwell’s equations, early introduced in James Clerk Maxwell’s paper [35], consist of four coupled vector partial-differential equations which describe all classical electromagnetic phenomena. In the MKS unit system, Maxwell’s equations in charge-free region are given in differential form by

\[
\frac{\partial B}{\partial t} = -\nabla \times E - M - \sigma E \quad \text{(Faraday’s law)},
\]

\[
\frac{\partial D}{\partial t} = \nabla \times H - J - \sigma^* H \quad \text{(Ampere’s law)},
\]

\[
\nabla \cdot D = 0 \quad \text{(Gauss’ law for the electric field)},
\]

\[
\nabla \cdot B = 0 \quad \text{(Gauss’ law for the magnetic field)},
\]

where \(E\) is the electric field, \(D\) is the electric flux density, \(H\) is the magnetic field, and \(B\) is the magnetic flux density. \(J\) and \(M\) are the independent sources of the electric and magnetic field energy, respectively, \(\sigma\) is the electric conductivity and \(\sigma^*\) is the equivalent magnetic loss. In this section, we will construct the electromagnetic formulation for the linear, isotropic, nondispersive materials, i.e., materials having field-independent, direction-independent, and
frequency-dependent. In other words, the relationships between electric field and electric flux density, magnetic field and magnetic flux density are described by

\[ D = \varepsilon E; \quad B = \mu H, \]  

(2.1.5)

where \( \varepsilon \) and \( \mu \) are, respectively, electrical permittivity and magnetic permeability.

By expanding the curl operators in (2.1.1) and (2.1.2) and employing the relations mentioned in (2.1.5), the system of six coupled scalar equations are obtained as follows

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

(2.1.6)

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

(2.1.7)

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

(2.1.8)

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

(2.1.9)

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

(2.1.10)

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

(2.1.11)

It is noted that the finite-difference time-domain (FDTD) methods only require the system of six coupled partial differential equations (2.1.6)–(2.1.11) to simulate electromagnetic wave interactions with general three dimensional objects. The Gauss’ laws relations in (2.1.3) and (2.1.4) are not explicitly enforced by the FDTD algorithms because they will be the consequences of the choice of the space lattice.

### 2.1.2 Reduction to two dimensions

In this thesis, we only focus on the two dimensional versions of Maxwell’s equations. We assume that the modeled structure can be extended to the infinity with no variations in the \( z \)-direction. Under that supposition, all partial derivatives of the fields with respect to \( z \)
must be equal to zero. As a result, the Maxwell’s equations (2.1.6)–(2.1.11) will be reduced to

\[
\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left( -\frac{\partial E_z}{\partial y} - M_x - \sigma^* H_x \right), \tag{2.1.12}
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - M_y - \sigma^* H_y \right), \tag{2.1.13}
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - M_z - \sigma^* H_z \right), \tag{2.1.14}
\]

\[
\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_z}{\partial y} - J_x - \sigma E_x \right), \tag{2.1.15}
\]

\[
\frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left( -\frac{\partial H_z}{\partial x} - J_y - \sigma E_y \right), \tag{2.1.16}
\]

\[
\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - J_z - \sigma E_z \right). \tag{2.1.17}
\]

We now group equations (2.1.12)–(2.1.17) according to field vector components. To be specific, we first group equations (2.1.12), (2.1.13), and (2.1.17) to form a set involving only \( H_x, H_y, \) and \( E_z \). We refer to this set as the transverse-magnetic mode with respect to \( z \) (TM\(_z\)). For another type of set, we group equations (2.1.14), (2.1.15), and (2.1.16), which involve only \( E_x, E_y, \) and \( H_z \). This set of field components is designated as the transverse-electric mode with respect to \( z \) (TE\(_z\)). The resulting sets of equations are given by

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

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_z}{\partial x} - M_y - \sigma^* H_y \right), \tag{2.1.18}
\]

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

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

\[ \frac{\partial E_y}{\partial t} = \frac{1}{\epsilon} \left( -\frac{\partial H_z}{\partial x} - J_y - \sigma E_y \right), \] \hspace{1cm} (2.1.19) \]

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

In source-free region (\( M = 0, J = 0 \)), and lossless materials (\( \sigma = 0, \sigma^* = 0 \)), we will obtain simpler forms for TM\(_z\) mode and TE\(_z\) mode. Under those assumptions and by considering non-magnetic materials, i.e. only permeability \( \mu \) is a time-independent function, Maxwell’s equations in 2D can be written as

\[ \frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \frac{\partial E_z}{\partial y}, \]

\[ \frac{\partial H_y}{\partial t} = \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \]

\[ \frac{\partial D_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}, \] \hspace{1cm} (2.1.20) \]

and

\[ \frac{\partial D_x}{\partial t} = \frac{\partial H_z}{\partial y}, \]

\[ \frac{\partial D_y}{\partial t} = -\frac{\partial H_z}{\partial x}, \]

\[ \frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right). \] \hspace{1cm} (2.1.21) \]

It can be seen that the TM\(_z\) and TE\(_z\) modes are independent of each other since they contain no common field components. For simple media like nondispersive media, the FDTD algorithms designed for the TM mode can be reused for the TE mode without any major modifications. However, for the complex media, the simulations for the different modes require different approaches. In general, the physical phenomena related to these two modes
can be dissimilar. This is because of the orientation of the electric and magnetic field vectors relative to the surface of the modeled structure. We can observe that in the TM$_z$ mode the direction of the electric components parallel the $z$–line of the structure. On the other hand, the $E$–field lines in the TE$_z$ mode belong to plane perpendicular to the $z$–axis of the structure.

### 2.1.3 Reduction to one dimension

From 2D case, we can further simplify Maxwell’s equations by assuming electromagnetic fields and system are invariant in the $y$–direction. That results in that all field partial derivatives in TM$_z$ and TE$_z$ modes w.r.t $y$ are equal to zero. We designate the 1D version of TM$_z$ mode as $x$–directed, $z$–polarized transverse electromagnetic (TEM) and 1D version of TE$_z$ mode as $x$–directed, $y$–polarized TEM. In the source-free region, and lossless materials, the simplest versions of TM$_z$ mode (2.1.18) and TE$_z$ mode (2.1.19) are given by

\[
\begin{align*}
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \frac{\partial H_y}{\partial x},
\end{align*}
\]

(2.1.22)

and

\[
\begin{align*}
\frac{\partial E_y}{\partial t} &= -\frac{1}{\epsilon} \frac{\partial H_z}{\partial x}, \\
\frac{\partial H_z}{\partial t} &= -\frac{1}{\mu} \frac{\partial E_y}{\partial x}.
\end{align*}
\]

(2.1.23)

### 2.2 Constitutive relations

This section introduces basic definition and general representations for both nondispersive and dispersive materials. The details of the constitutive relations for three common dispersive media including Debye, Drude, and Lorentz media are presented.
2.2.1 Definition

The constitutive relations relate the electric flux density $D$ to the electric intensity $E$, and similarly the magnetic flux density $B$ to the magnetic intensity $H$. The precise form of the constitutive relations depends on the type of the material. For example, in vacuum, they receive the simplest form

$$D = \epsilon_0 E, \quad B = \mu_0 H,$$

(2.2.1)

where $\epsilon_0 = 8.854 \times 10^{-12}$ farads/meter is the free-space permittivity, and $\mu_0 = 4\pi \times 10^{-7}$ henrys/meter is the free-space permeability.

2.2.2 Nondispersive materials

A nondispersive material refers to a material having time-independent constitutive relations. In other word, the field intensities and their flux densities are related by scalar constants as follows

$$D = \epsilon_r \epsilon_0 E, \quad B = \mu_r \mu_0 H,$$

(2.2.2)

where $\epsilon_r$ and $\mu_r$ are, respectively, the relative permittivity and permeability.

2.2.3 Dispersive materials

In dispersive materials, permittivity and permeability are functions of frequency. Therefore, for linear, isotropic materials, their constitutive relations can be represented as the following harmonic-form

$$\hat{D}(\omega) = \hat{\epsilon}(\omega)\hat{E}(\omega), \quad \hat{B}(\omega) = \hat{\mu}(\omega)\hat{H}(\omega),$$

(2.2.3)
where $\epsilon$ and $\mu$ are the permittivity and permeability, respectively, $\omega$ is angular frequency, and a caret denotes a quantity in a frequency domain. There are three important generic classes of linear, isotropic, dispersive materials, namely, Debye materials, Drude materials, and Lorentz materials. In those media, the permeability $\mu$ is just a scalar constant, while the permittivity $\epsilon$ is a complex number. The following are the representations of the permittivity for each type of media having $P$ poles

- **Debye media**
  \[
  \epsilon(\omega) = \epsilon_0 \left( \epsilon_\infty + \sum_{p=1}^{P} \frac{\epsilon_{s,p} - \epsilon_\infty}{1 + j\omega\gamma_p} \right),
  \]
  \[\text{(2.2.4)}\]
  where $\epsilon_{s,p}$ and $\epsilon_\infty$ are, respectively, the permittivities at static frequency, and at high frequency limit. Here $j$ is the imaginary unit, and $\gamma$ is the relaxation time constant.

- **Drude media**
  \[
  \epsilon(\omega) = \epsilon_0 \left( \epsilon_\infty - \sum_{p=1}^{P} \frac{\omega_p^2}{\omega^2 - j\omega\gamma_p} \right),
  \]
  \[\text{(2.2.5)}\]
  where $\omega_p$ is the frequency of the pole pair.

- **Lorentz media**
  \[
  \epsilon(\omega) = \epsilon_0 \left( \epsilon_\infty + \sum_{p=1}^{P} \frac{(\epsilon_{s,p} - \epsilon_\infty) \omega_p^2}{\omega_p^2 + 2j\omega\sigma_p - \omega^2} \right),
  \]
  \[\text{(2.2.6)}\]
  where $\sigma_p$ is the damping coefficient.

### 2.3 Auxiliary differential equation method

We see that the constitutive relations for the dispersive media are represented in the frequency-domain, but Maxwell’s equations (2.1.1)–(2.1.2) are declared in the time-domain. Therefore, there is a need of employing a so-called auxiliary differential equation (ADE) method [18, 36] to express the relationship between $\mathbf{D}$ and $\mathbf{E}$ in a differential equation form rather than the convolution integral form. An alternative technique to implement the constitutive relations in the dispersive media has been developed by Luebbers et al. [37], known as piecewise-linear recursive-convolution method (PLRC). Both ADE and PLRC
methods have same second-order accuracy; however, ADE methods are more attractive since they can be employed to model the arbitrary nonlinear dispersive media. In addition, since there is no need to use of complex-number arithmetic in the ADE approach, this method requires fewer floating-point operations, and an equal or smaller number of unknowns to be stored in the memory than its counterpart [36]. The main idea of the ADE method is to take the inverse Fourier transformation of the relationship between $D$ and $E$ in (2.2.3), and transform back to the time-domain by noticing that a multiplication with $j\omega$ as a first-order derivative in time, and a multiplication with $(j\omega)^2 = -\omega$ as a second-order derivative in time [38]. In the rest of this section, we will discuss the ADE technique separately for Debye, Drude, and Lorentz materials. For simplicity, only single-pole models are taken into account.

2.3.1 Single-order Debye dispersion model

According to (2.2.4), the single-pole Debye medium (i.e, $P = 1$) has the following form

with neglect of the subscript $p$ for convenience

$$\hat{D}(\omega) = \epsilon_0 \left( \epsilon_\infty + \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega \gamma} \right) \hat{E}(\omega), \quad (2.3.1)$$

algebra simplications give us that

$$\left(1 + j\omega \gamma\right) \hat{D}(\omega) = \epsilon_0 \epsilon_s \hat{E}(\omega) + j\omega \gamma \epsilon_0 \epsilon_\infty, \quad (2.3.2)$$

taking the inverse Fourier transformation of equation (2.3.2) to get

$$D + \gamma \frac{\partial D}{\partial t} = \epsilon_0 \epsilon_s E + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t}, \quad (2.3.3)$$
write out the vector components of (2.3.3), we achieve
\[ D_w + \gamma \frac{\partial D_w}{\partial t} = \epsilon_0 \epsilon_s E_w + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E_w}{\partial t}, \quad \text{for} \ w = x, y, \text{and} \ z. \quad (2.3.4) \]

### 2.3.2 Single-order Drude dispersion model

By taking \( P = 1 \) in (2.2.5), and denoting \( \epsilon_s := \epsilon_{s,1} \) and \( \gamma := \gamma_1 \), the relationship of \( D \) and \( E \) in the single-pole Drude medium is given by
\[ \hat{D}(\omega) = \epsilon_0 \left( \epsilon_\infty - \frac{\omega_1^2}{\omega^2 - j\omega \gamma} \right) \hat{E}(\omega), \quad (2.3.5) \]
removing the fraction form to find
\[ \omega^2 \hat{D}(\omega) - j\omega \hat{D}(\omega) = \epsilon_0 \epsilon_\infty \omega^2 \hat{E}(\omega) - \epsilon_0 \epsilon_\infty \gamma j\omega \hat{E}(\omega) - \epsilon_0 \omega_1^2 \hat{E}(\omega), \quad (2.3.6) \]

The inverse Fourier transformation is again used to convert the harmonic equation into the time domain
\[ \frac{\partial^2 D}{\partial t^2} + \gamma \frac{\partial D}{\partial t} = \epsilon_0 \epsilon_\infty \frac{\partial^2 E}{\partial t^2} + \epsilon_0 \epsilon_\infty \gamma \frac{\partial E}{\partial t} + \epsilon_0 \omega_1^2 E, \quad (2.3.7) \]

### 2.3.3 Single-order Lorentz dispersion model

Finally, for a completeness, we present the ADE approach for the Lorentz media. The first pole representation in (2.2.6) gives rise
\[ D(\omega) = \epsilon_0 \left( \epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)\omega_1^2}{\omega_1^2 + 2j\omega \sigma_1 - \omega^2} \right) E(\omega), \quad (2.3.8) \]
canceling the denominator of (2.3.8) to achieve
\[
\omega_1^2 \mathbf{D}(\omega) + 2j\omega\sigma_1 \mathbf{D}(\omega) - \omega^2 \mathbf{D}(\omega) = \epsilon_0 \epsilon_\infty \omega_1^2 \mathbf{E}(\omega) + 2\epsilon_0 \epsilon_\infty \sigma_1 j\omega \mathbf{E}(\omega) - \epsilon_0 \epsilon_\infty \omega^2 \mathbf{E}(\omega)
\]
\[+ \epsilon_0 (\epsilon_s - \epsilon_\infty) \omega_1^2 \mathbf{E}(\omega), \quad (2.3.9)\]

thanks to the inverse Fourier transformation, the time-domain version of the constitutive relation for Lorentz media is attained as follows
\[
\frac{\partial^2 \mathbf{D}}{\partial t^2} + 2\sigma_1 \frac{\partial \mathbf{D}}{\partial t} + \omega_1^2 \mathbf{D} = \epsilon_0 \epsilon_\infty \frac{\partial^2 \mathbf{E}}{\partial t^2} + 2\sigma_1 \epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} + \epsilon_0 \epsilon_s \omega_1^2 \mathbf{E}, \quad (2.3.10)
\]

### 2.4 Time-stepping scheme for Maxwell system

This section briefly introduces three common classes of time-stepping methods, namely first-order Euler method, leapfrog method, and Runge-Kutta methods, which can be used to discretize the time derivatives in Maxwell’s equations. To illustrate the approach of each type of method, we shall consider \(x\)--directed, \(z\)--polarized TEM described at (2.1.22) for simplicity. At a discrete time \(t_n = n\Delta t\) with \(\Delta t\) is the time increment, the function value at that time point and grid position \(x\) is defined as \(y(t_n, x)\).

#### 2.4.1 First-order Euler method

This method discretizes the time derivative of \(y(t, x)\) as
\[
\frac{\partial y(t, x)}{\partial t} = \frac{y(t + \Delta t, x) - y(t, x)}{\Delta t} + O(\Delta t).
\] (2.4.1)
Note that the approximation in (2.4.1) is only first-order accuracy. We then approximate
the time derivatives of Eqs. (2.1.22) at \( t_n \) in a manner as (2.4.1) to arrive at

\[
\frac{H_y(t_{n+1}, x) - H_y(t_n, x)}{\Delta t} \approx \frac{1}{\mu} \frac{\partial E_z}{\partial x}(t_n, x),
\]  
\( \text{(2.4.2)} \)

\[
\frac{E_z(t_{n+1}, x) - E_z(t_n, x)}{\Delta t} \approx \frac{1}{\epsilon} \frac{\partial H_y}{\partial x}(t_n, x).
\]  
\( \text{(2.4.3)} \)

Simplifying above equations to get the values of electromagnetic fields at \( t_{n+1} \)

\[
H_y(t_{n+1}, x) \approx H_y(t_n, x) + \frac{\Delta t}{\mu} \frac{\partial E_z}{\partial x}(t_n, x),
\]  
\( \text{(2.4.4)} \)

\[
E_z(t_{n+1}, x) \approx E_z(t_n, x) + \frac{\Delta t}{\epsilon} \frac{\partial H_y}{\partial x}(t_n, x).
\]  
\( \text{(2.4.5)} \)

One should keep in mind that the spatial discretization will not be discussed in this
section but will be given explicitly in Section 2.5.

2.4.2 The leapfrog method

The leapfrog method was first appeared in [39] to solve the parabolic partial differential
equations (PDEs). Unfortunately, it turns out that this method renders solutions of this
class of PDEs unstable results. However, it well servers the hyperbolic PDEs which are the
forms of most electromagnetic problems. Unlike the first-order Euler method, the leapfrog
scheme discretizes the time derivative of function value \( y(t, x) \) in a time-centered manner.
This approach gives rise to the following approximation

\[
\frac{\partial y}{\partial t}\left(t + \frac{\Delta t}{2}, x\right) = \frac{y(t + \Delta t, x) - y(t, x)}{\Delta t} + O(\Delta t^2).
\]  
\( \text{(2.4.6)} \)

Notice that the right hand side of (2.4.6) is the same as the one of (2.4.1) in the Euler
method, but the left hand side of (2.4.6) is evaluated at \( t + \frac{\Delta t}{2} \) instead of at \( t \). Therefore, a
second-order accuracy is attained for the leapfrog scheme.
In order to discretize the time derivatives of TEM mode (2.1.22) in the leapfrog manner, the time positions of \( E_z \) and \( H_y \) have to be placed in a staggered fashion. In particular, \( E_z \) will be evaluated at \( t_n \) while \( H_y \) will be determined at \( t_{n+\frac{1}{2}} = t_n + \frac{\Delta t}{2} \). By applying the leapfrog scheme for the first equation at \( t_{n+1} \) and for the second equation at \( t_{n+\frac{1}{2}} \) in (2.1.22), one gets

\[
\frac{E_z(t_{n+1}, x) - E_z(t_n, x)}{\Delta t} \approx \frac{1}{\epsilon} \frac{\partial H_y}{\partial x}(t_{n+\frac{1}{2}}, x), \quad (2.4.7)
\]
\[
\frac{H_y(t_{n+\frac{3}{2}}, x) - H_y(t_{n+\frac{1}{2}}, x)}{\Delta t} \approx \frac{1}{\mu} \frac{\partial E_z}{\partial x}(t_{n+1}, x). \quad (2.4.8)
\]

Arranging the above equations, one achieves

\[
E_z(t_{n+1}, x) \approx E_z(t_n, x) + \frac{\Delta t}{\epsilon} \frac{\partial H_y}{\partial x}(t_{n+\frac{1}{2}}, x), \quad (2.4.9)
\]
\[
H_y(t_{n+\frac{3}{2}}, x) \approx H_y(t_{n+\frac{1}{2}}, x) + \frac{\Delta t}{\mu} \frac{\partial E_z}{\partial x}(t_{n+1}, x). \quad (2.4.10)
\]

The leapfrog approach is common use in the computational electromagnetics because it is a second-order, fully explicit and conditional stable method. Another advantages of this scheme will be insightfully discussed in Section 2.5

2.4.3 Runge-Kutta methods

In two previously introduced methods, the first-order Euler method is the simplest way to approximate the time-derivative but only exhibits first-order accuracy. Since the leapfrog method has second-order accuracy, it is commonly used as time-stepping scheme for most hyperbolic PDEs. However, if one requires a higher order accuracy for the time discretization, the forth order Runge-Kutta scheme, or RK4, is an ideal choice. Let \( Q^n = (E_z(x_1, t_n), \ldots, E_z(x_N, t_n), H_y(\bar{x}_1, t_n), \ldots, H_y(\bar{x}_N, t_n)) \). Where \( N \) is the total number of grid points for either \( E_z \) or \( H_y \), \( x_k \) and \( \bar{x}_k \) \((k = 1, \ldots, N)\) are grid positions for \( E_z \) and \( H_y \), re-
spectively. By letting $S$ be the spatial discretization of the left hand sides in TEM mode (2.1.22), we obtain the following semi-discretization

$$\frac{\partial Q^n}{\partial t} = \frac{1}{\Delta x} SQ^n,$$

(2.4.11)

where $\Delta x$ is the spatial increment.

With given data at a discrete time $t_n$, the forecast values of the electromagnetic components are determine via the following RK4 process [26, 40] as

$$Q^{n+1} = Q^n + \frac{\Delta t}{6} (K_1 + 2K_2 + 2K_3 + K_4),$$

(2.4.12)

with

$$K_1 = \frac{\Delta t}{\Delta x} SQ^n,$$

(2.4.13)

$$K_2 = \frac{\Delta t}{\Delta x} S\left(Q^n + \frac{1}{2} K_1\right),$$

(2.4.14)

$$K_3 = \frac{\Delta t}{\Delta x} S\left(Q^n + \frac{1}{2} K_2\right),$$

(2.4.15)

$$K_4 = \frac{\Delta t}{\Delta x} S\left(Q^n + K_3\right).$$

(2.4.16)

It is reported that the stability region of RK4 method is bigger than that of the leapfrog scheme (see Section 2.5.5). However, RK4 process consumes more CPU time than the second-order method (see CPU time reports in the numerical experiment Sections of Chapters 5 and 6).

### 2.5 The Yee Algorithm

In this section, a brief history and some noteworthy features of the Yee scheme is presented in the introduction part. The details of the Yee approach for different materials are presented. A concise stability discussion ends this section.
2.5.1 Introduction

The classical finite-different time-domain method (FDTD), or Yee scheme, for the time-dependent Maxwell’s curl equations system of (2.1.1) and (2.1.2) in free space was firstly designed by Yee in 1966 [41]. In the Yee algorithm, the electric and magnetic fields are both solved by discretizing the coupled Maxwell’s equations instead of solving separately the field components in wave equations. Furthermore, the Yee scheme suggests using the staggered-grid to enhance the stability. To illustrate this grid type, we consider field allocations for the TM$_z$ mode in source-free region and lossless materials. In this mode, the staggered-grid will place the $E_z$ component in a center surrounded by the magnetic components $H_x$ and $H_y$, see Fig. 2.1. The most important attribute of this space lattice is to implicitly enforce the divergence-free conditions, see Section 2.5.4. For the time allotment, the Yee scheme also centers its electric and magnetic components in a leapfrog manner. The time-space chart of the Yee algorithm is depicted in Fig. 2.1. The use of this time-stepping scheme allows us to explicitly solve Maxwell’s equations; therefore, the involvement with simultaneous equations and matrix inversion is evaded.

Figure 2.1: Time position chart and staggered grid system of the Yee scheme for the TM$_z$ mode. Left: time positions. Right: staggered grid system.
2.5.2 Finite-different time-domain (FDTD) method for nondispersive materials

For the convenience of demonstrating the Yee scheme, we adopt the following notations

\[(i, j) = (i \Delta x, j \Delta y), \quad t_n = n \Delta t, \quad (2.5.1)\]

and

\[\left( i + \frac{1}{2}, j + \frac{1}{2} \right) = \left( i + \frac{1}{2} \right) \Delta x, \left( j + \frac{1}{2} \right) \Delta y, \quad t_{n+\frac{1}{2}} = \left( n + \frac{1}{2} \right) \Delta t, \quad (2.5.2)\]

where \(\Delta x\), and \(\Delta y\) are, respectively, the lattice space increment along the \(x\) and \(y\) directions, and \(i, j\) are integers. \(\Delta t\) is the time increment, and \(n\) is integer. In addition, the function value \(u\) defined at a discrete position in grid \((i \Delta x, j \Delta y)\) and a discrete point in time \(n \Delta t\) is denoted as

\[u(i \Delta x, j \Delta y, n \Delta t) = u^n_{i,j}. \quad (2.5.3)\]

The idea of Yee scheme is to use the leapfrog approximation \((2.4.6)\) for both spatial and temporal discretizations. The \(x\) derivative of any field component at mesh point \((i, j)\) and time point \(n \Delta t\), thus, is given as

\[\frac{\partial u}{\partial x}\bigg|_{i,j}^n \approx \frac{u^n_{i+\frac{1}{2},j} - u^n_{i-\frac{1}{2},j}}{\Delta x}, \quad (2.5.4)\]

time derivative at time step \(n\)

\[\frac{\partial u}{\partial t}\bigg|_{i,j}^n \approx \frac{u^{n+\frac{1}{2}}_{i,j} - u^{n-\frac{1}{2}}_{i,j}}{\Delta t}, \quad (2.5.5)\]
and a semi-implicit approximation is defined as
\[
|u|_{i,j}^n \approx \frac{|u|_{i,j}^{n+\frac{1}{2}} + |u|_{i,j}^{n-\frac{1}{2}}}{2}.
\] (2.5.6)

We first consider Yee's approach to discretize 2D Maxwell's equations in source-free region with lossless, homogeneous, isotropic materials. In particular, the following systems are taken into account

\[
\begin{align*}
\frac{\partial H_x}{\partial t} &= -\frac{1}{\mu} \frac{\partial E_z}{\partial y}, \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right),
\end{align*}
\] (2.5.7)

and

\[
\begin{align*}
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon} \frac{\partial H_z}{\partial y}, \\
\frac{\partial E_y}{\partial t} &= -\frac{1}{\epsilon} \frac{\partial H_z}{\partial x}, \\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right).
\end{align*}
\] (2.5.8)

Since the FDTD expressions for various modes do not yield any major differences in this case, we only mention the finite-difference forms for the TM mode. Discretizing (2.5.7) in
the same manners as in (2.5.4) to achieve

\[
\frac{\partial H_x}{\partial t} \bigg|_{i,j+\frac{1}{2}}^n = -\frac{1}{\mu} \left( \frac{E_z|_{i,j+1}^n - E_z|_{i,j-1}^n}{\Delta y} \right),
\]

(2.5.9)

\[
\frac{\partial H_y}{\partial t} \bigg|_{i+\frac{1}{2},j}^n = \frac{1}{\mu} \left( \frac{E_z|_{i+1,j}^n - E_z|_{i,j}^n}{\Delta x} \right),
\]

(2.5.10)

\[
\frac{\partial E_z}{\partial t} \bigg|_{i,j}^{n+\frac{1}{2}} = \frac{1}{\epsilon} \left( \frac{H_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j}^{n+\frac{1}{2}}}{\Delta x} - \frac{H_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y} \right).
\]

(2.5.11)

Next, by applying (2.5.5) to time derivative in the above spatial discretized system, we finally attain the Yee algorithm for the TM mode

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

(2.5.12)

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

(2.5.13)

\[
E_z|_{i,j}^{n+1} = E_z|_{i,j}^n + \frac{\Delta t}{\epsilon} \left( \frac{H_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j}^{n+\frac{1}{2}}}{\Delta x} - \frac{H_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y} \right).
\]

(2.5.14)

In the inhomogeneous materials, the medium parameters \((\epsilon, \mu)\) will change throughout the computational domain. Consequently, the Yee scheme will be modified slightly as

\[
H_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} = H_x|_{i,j+\frac{1}{2}}^{n-\frac{1}{2}} - \frac{\Delta t}{\mu_{i,j+\frac{1}{2}} \Delta y} \left( E_z|_{i,j+1}^n - E_z|_{i,j-1}^n \right),
\]

(2.5.15)

\[
H_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} = H_y|_{i+\frac{1}{2},j}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_{i+\frac{1}{2},j} \Delta y} \left( E_z|_{i+1,j}^n - E_z|_{i-1,j}^n \right),
\]

(2.5.16)

\[
E_z|_{i,j}^{n+1} = E_z|_{i,j}^n + \frac{\Delta t}{\epsilon_{i,j}} \left( \frac{H_y|_{i+\frac{1}{2},j}^{n+\frac{1}{2}} - H_y|_{i-\frac{1}{2},j}^{n+\frac{1}{2}}}{\Delta x} - \frac{H_x|_{i,j+\frac{1}{2}}^{n+\frac{1}{2}} - H_x|_{i,j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta y} \right).
\]

(2.5.17)
The numerical discretizations (2.5.15), (2.5.16), and (2.5.17) are useful to simulate the interface problems. However, this approach only gives us first-order accuracy when medium parameters \((\epsilon, \mu)\) are discontinuous in the simulation space.

### 2.5.3 FDTD method for dispersive materials

In this subsection, we only describe the FDTD scheme for the TM\(_z\) mode because similar finite-difference expressions will be conducted for the TE\(_z\) mode. We first consider Maxwell’s equations involving Debye media formed by Eqs. (2.1.20) and relations (2.3.4). That gives rise to following system of equations

\[
\begin{align*}
\frac{\partial H_x}{\partial t} &= -\epsilon \frac{\partial E_z}{\partial y}, \\
\frac{\partial H_y}{\partial t} &= \epsilon \frac{\partial E_z}{\partial x}, \\
\frac{\partial D_z}{\partial t} &= \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}, \\
D_z + \gamma \frac{\partial D_z}{\partial t} &= \epsilon_0 \epsilon_s E_z + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E_z}{\partial t}.
\end{align*}
\]

(2.5.18) (2.5.19) (2.5.20) (2.5.21)

In comparison to the Maxwell’s equations for nondispersive materials (2.5.9)–(2.5.11), the system (2.5.18)–(2.5.21) comprises an additional constitutive relation which is Eq. (2.5.21). This equation can be discretized in the same manner as in (2.5.5) and (2.5.6). Using this strategy, we write the following finite-difference expression for (2.5.21) at \(n + \frac{1}{2}\)

\[
\begin{align*}
D_z^n_{i,j} + \frac{\gamma}{2} \frac{D_z^{n+\frac{1}{2}}_{i,j}}{\mu} + \gamma \frac{E_z^{n+\frac{1}{2}}_{i,j}}{\epsilon_\infty} \frac{\partial E_z}{\partial t}^{n+\frac{1}{2}}_{i,j} &= \epsilon_0 \epsilon_s E_z^n_{i,j} + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E_z}{\partial t}^n_{i,j}, \\
\frac{D_z^{n+1}_{i,j} + D_z^n_{i,j}}{2} + \gamma \frac{D_z^{n+1}_{i,j} - D_z^n_{i,j}}{\Delta t} &= \epsilon_0 \epsilon_s E_z^{n+1}_{i,j} + \frac{E_z^n_{i,j}}{2} \\
&+ \gamma \epsilon_0 \epsilon_\infty \frac{E_z^{n+1}_{i,j} - E_z^n_{i,j}}{\Delta t}.
\end{align*}
\]

(2.5.22) (2.5.23)
A value of $E_z$ at time step $n + 1$ can be updated via Eq. (2.5.23). As a result, we arrive at a complete Yee algorithm for the Debye media

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

(2.5.24)

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

(2.5.25)

\[
D_z^{n+1} = D_z^n + \Delta t \left( \frac{H_y^{n+\frac{1}{2}} - H_y^{n-\frac{1}{2}}}{\Delta x} - \frac{H_x^{n+\frac{1}{2}} - H_x^{n-\frac{1}{2}}}{\Delta y} \right),
\]

(2.5.26)

\[
E_z^{n+1} = \left( \frac{\Delta t + 2\gamma}{\Delta t \epsilon_0 \epsilon_s + 2\gamma \epsilon_0 \epsilon_\infty} \right) D_z^{n+1} + \left( \frac{\Delta t - 2\gamma}{\Delta t \epsilon_0 \epsilon_s + 2\gamma \epsilon_0 \epsilon_\infty} \right) D_z^n + \left( -\Delta t \epsilon_0 \epsilon_s + 2\gamma \epsilon_0 \epsilon_\infty \right) E_z^n.
\]

(2.5.27)

We next examine a Drude dispersive medium having one pole in its susceptibility response. The constitutive relation in the TM$_z$ for this medium is given by considering $z$ component of (2.3.7)

\[
\frac{\partial^2 D_z}{\partial t^2} + \gamma \frac{\partial D_z}{\partial t} = \epsilon_0 \epsilon_\infty \frac{\partial^2 E_z}{\partial t^2} + \epsilon_0 \epsilon_\infty \gamma \frac{\partial E_z}{\partial t} + \epsilon_0 \omega_1^2 E_z,
\]

(2.5.28)

We can now evaluate (2.5.28) at time step $n$ and at grid node $(i,j)$, to get

\[
\left. \frac{\partial^2 D_z}{\partial t^2} \right|_{i,j}^{n} + \gamma \left. \frac{\partial D_z}{\partial t} \right|_{i,j}^{n} = \epsilon_0 \epsilon_\infty \left. \frac{\partial^2 E_z}{\partial t^2} \right|_{i,j}^{n} + \epsilon_0 \epsilon_\infty \gamma \left. \frac{\partial E_z}{\partial t} \right|_{i,j}^{n} + \epsilon_0 \omega_1^2 E_z^n.
\]

(2.5.29)

By discretizing time derivatives in the leapfrog manner, we attain

\[
\frac{D_z^{n+1}_{i,j} - 2 D_z^n_{i,j} + D_z^{n-1}_{i,j}}{\Delta t^2} + \gamma \frac{D_z^{n+1}_{i,j} - D_z^{n-1}_{i,j}}{2\Delta t} = \epsilon_0 \epsilon_\infty \frac{E_z^{n+1}_{i,j} - 2 E_z^n_{i,j} + E_z^{n-1}_{i,j}}{\Delta t^2}
\]

\[
+ \epsilon_0 \epsilon_\infty \gamma \frac{E_z^{n+1}_{i,j} - E_z^{n-1}_{i,j}}{2\Delta t} + \epsilon_0 \omega_1^2 E_z^n._{i,j},
\]

(2.5.30)
Solving (2.5.30) for $E_z|_{i,j}^{n+1}$, we get

$$E_z|_{i,j}^{n+1} = C_1^D D_z|_{i,j}^{n+1} + C_2^D D_z|_{i,j}^{n} + C_3^D D_z|_{i,j}^{n-1} + C_4^D E_z|_{i,j}^{n} + C_5^D E_z|_{i,j}^{n-1}, \quad (2.5.31)$$

where

$$C_1^D = \frac{1}{\epsilon_0 \epsilon_\infty}, \quad C_2^D = \frac{-4}{(2 + \gamma \Delta t) \epsilon_0 \epsilon_\infty}, \quad C_3^D = \frac{2 - \gamma \Delta t}{\epsilon_0 \epsilon_\infty (2 + \gamma \Delta t)}, \quad C_4^D = \frac{4 \epsilon_\infty - \omega_1^2 \Delta t^2}{(2 + \gamma \Delta t) \epsilon_\infty},$$

$$C_5^D = \frac{\gamma \Delta t - 2}{\gamma \Delta t + 2}.$$

One can achieve a Yee algorithm for Maxwell’s equations with Drude dispersive media by employing discretizations (2.5.24), (2.5.25) and (2.5.26) to update values for $H_x$, $H_y$ and $D_z$, respectively. Finally, the updated value for $E_z$ is deduced via (2.5.31). Note that unlike the Debye media, the Drude media features a second-order time-derivative at the constitutive relation; consequently, the evaluation of $E_z$ at time step $n + 1$ requires two previous field data at $n$ and $n - 1$.

Finally, at the risk of repetitiveness, we will present the FDTD expressions for the Lorentz media. In the TM$_z$ mode, the Lorentz constitutive relation is attained by projecting (2.3.10) along the $z-$direction resulting in the following relationship

$$\frac{\partial^2 D_z}{\partial t^2} + 2\sigma_1 \frac{\partial D_z}{\partial t} + \omega_1^2 D_z = \epsilon_0 \epsilon_\infty \frac{\partial^2 E_z}{\partial t^2} + 2\sigma_1 \epsilon_0 \epsilon_\infty \frac{\partial E_z}{\partial t} + \epsilon_0 \epsilon_s \omega_1^2 E_z. \quad (2.5.32)$$

Similarly to the Drude case, this media also exhibits a second-order ODE at the constitutive relation; therefore, the predicted value will rely on at least two previous time-step field components. Indeed, evaluating (2.5.32) at a discrete time $t_n$ and at grid point $(i,j)$, to get

$$\frac{D_z|_{i,j}^{n+1} - 2 D_z|_{i,j}^{n} + D_z|_{i,j}^{n-1}}{\Delta t^2} + 2\sigma_1 \frac{D_z|_{i,j}^{n+1} - D_z|_{i,j}^{n-1}}{2\Delta t} + \omega_1^2 D_z|_{i,j}^{n} = \epsilon_0 \epsilon_\infty \frac{E_z|_{i,j}^{n+1} - 2 E_z|_{i,j}^{n} + E_z|_{i,j}^{n-1}}{\Delta t^2} + 2\sigma_1 \epsilon_0 \epsilon_\infty \frac{E_z|_{i,j}^{n+1} - E_z|_{i,j}^{n-1}}{2\Delta t} + \epsilon_0 \epsilon_s \omega_1^2 E_z|_{i,j}^{n}. \quad (2.5.33)$$
Solving (2.5.33) for \( E_{z|_{i,j}}^{n+1} \), one obtains

\[
E_{z|_{i,j}}^{n+1} = C_1^L D_{z|_{i,j}}^{n+1} + C_2^L D_{z|_{i,j}}^{n} + C_3^L D_{z|_{i,j}}^{n-1} + C_4^L E_{z|_{i,j}}^{n} + C_5^L E_{z|_{i,j}}^{n+1},
\]

(2.5.34)

where

\[
C_1^L = \frac{1}{\epsilon_0 \epsilon_\infty}, \quad C_2^L = \frac{-2 + \Delta t^2 \omega_1^2}{\epsilon_0 \epsilon_\infty (1 + \sigma_1 \Delta t)}, \quad C_3^L = \frac{1 - \sigma_1 \Delta t}{\epsilon_0 \epsilon_\infty (1 + \sigma_1 \Delta t)},
\]

\[
C_4^L = \frac{2 \epsilon_\infty - \epsilon_\infty \omega_1^2 \Delta t^2}{\epsilon_\infty (1 + \sigma_1 \Delta t)}, \quad C_5^L = \frac{-1 + \sigma_1 \Delta t}{1 + \sigma_1 \Delta t}.
\]

The found of discretization (2.5.34) along with the mentioned finite-difference expressions at (2.5.25) and (2.5.26) give us a Yee approach for Maxwell’s equations in the Lorentz media.

### 2.5.4 Divergence-free nature

As already mentioned in the introduction part of the Yee algorithm, one significant advantage of the use of the staggered grid is to implicitly enforce the Gauss’ laws for the electric and magnetic fields. That implies our fields are divergence-free. To verify this statement, we will prove the Gauss’ law for the magnetic component will hold for the TM\(_z\) mode in the lossless, homogeneous space and source-free region. The Gauss’ law for the electric field can be likewise testified in the TE\(_z\) mode. By considering the integral form of relation (2.1.4), we have to show that

\[
\oint_S \mathbf{B} \cdot d\mathbf{S} = 0,
\]

(2.5.35)

where \( S \) is a closed rectangular surface, and \( dS \) is always outward from the surface. Since in the TM\(_z\) mode, the structure is invariant along the \( z \)-axis, we only evaluate the surface integral (2.5.35) on unit rectangle having sides \( \Delta x, \Delta z \) and \( \Delta y, \Delta z \) as shown in Fig. 2.2 to get
Figure 2.2: FDTD grid for verifying the divergence-free in the TM\textsubscript{z} mode.

\[
\oint_S \mathbf{B} \cdot d\mathbf{S} = \mu \left( H_x|^{i+1,j+\frac{1}{2}}_i - H_x|^{i+\frac{1}{2},j}_i \right) \Delta y \Delta z + \mu \left( H_y|^{i+\frac{1}{2},j+1}_i - H_y|^{i+1,j+\frac{1}{2}}_i \right) \Delta x \Delta z. \quad (2.5.36)
\]

Taking the time derivative of (2.5.36), and employing (2.5.9) and (2.5.10), one attains

\[
\frac{\partial}{\partial t} \oint_S \mathbf{B} \cdot d\mathbf{S} = \left( - E_z|^{i+1,j+1}_i + E_z|^{i+1,j}_i + E_z|^{i,j+1}_i + E_z|^{i,j}_i \right) \Delta z \\
+ \left( E_z|^{i+1,j+1}_i - E_z|^{i+1,j}_i - E_z|^{i,j+1}_i + E_z|^{i,j}_i \right) \Delta z = 0. \quad (2.5.37)
\]

Thus, for all time-steps, we always achieve

\[
\frac{\partial}{\partial t} \oint_S \mathbf{B} \cdot d\mathbf{S} = 0. \quad (2.5.38)
\]

The result at (2.5.38) implies that if the magnetic fields at the initial time satisfy the divergence-free condition, the Yee expressions will automatically enforce the the Gauss’ law.
for magnetic field in all computations.

### 2.5.5 Courant-Friedrichs-Lewy condition

The Courant-Friedrichs-Lewy (CFL) condition is a necessary condition for the convergence of the FDTD methods for solving PDEs problems. This condition is named after Richard Courant, Kurt Friedrichs, and Hans Lewy who introduced this condition in their paper [42]. In general, the CFL condition is stated that

\[
C = \Delta t \sum_{i=1}^{3} \frac{v_{x_i}}{\Delta x_i} \leq C_{\text{max}},
\]

(2.5.39)

where dimensionless \( C \) and \( C_{\text{max}} \) are the Courant number, \( v_{x_i} \) is the magnitude of the velocity for the corresponding direction. In practice, \( C_{\text{max}} \) can be called the CFL number.

The CFL condition for the Yee scheme in the free-space is described as [43]

\[
c\Delta t \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}} \leq 1,\]

(2.5.40)

where \( c = 1/\sqrt{\mu\varepsilon} \) is the speed of light in the material being modeled. This result indicates that the CFL number of the Yee scheme is 1. While keeping the spatial discretizations as in the Yee expressions, but the temporal discretization is carried out by the fourth-order Runge-Kutta method. This approach yields a CFL number is as high as \( \sqrt{2} \) [26].

### 2.6 Interface conditions and Perfect electric conductor

Along the interface involving two dissimilar media, the wave solutions could reduce their regularities and their manners across the interface are regulated by the interface conditions. If we consider an interface \( \Gamma \) with no sources or changes along it separating two materials as shown in Fig. 2.3, then the general interface conditions relate analytically the field solutions in both media having finite conductivity as [44]

28
\[ \vec{n} \times (E^+ - E^-) = 0, \quad \vec{n} \cdot (D^+ - D^-) = 0, \]
\[ \vec{n} \times (H^+ - H^-) = 0, \quad \vec{n} \cdot (B^+ - B^-) = 0, \]  
(2.6.1)

where \( \vec{n} \) is the unit vector pointing from \( \Omega^- \) to \( \Omega^+ \), and the superscript \(-\), or \(+\) denotes the limiting value of a function from the corresponding side of the interface.

When a medium has infinite electric conductivity, i.e \( \sigma = \infty \), it is called the perfect electric conductor (PEC). In this case, the interface \( \Gamma \) is referred to as a PEC wall, and denoted by \( \Gamma_{\text{PEC}} \). Since the PEC has a zero resistivity, the electric field at the PEC wall is vanish. By assuming one of the media being PEC, one gets following interface conditions \([44, 45]\)

\[ \vec{n} \times E = 0, \quad \vec{n} \cdot D = q_{es}, \]
\[ \vec{n} \times H = J_s, \quad \vec{n} \cdot B = 0, \]  
(2.6.2)

where \( q_{es} \) and \( J_s \) are, respectively, surface electric charge density and induced linear electric current density. We drop the superscripts \(+\) and \(-\) in the above because we are now left with the field components in the non-PEC side. In addition, these nonzero values are often unknown for the general problems. Therefore, the interface conditions related to these
unknown values are regularly omitted [45]; that results in reduced interface conditions on PEC

\[ \hat{n} \times \mathbf{E} = 0, \quad \hat{n} \cdot \mathbf{B} = 0. \tag{2.6.3} \]

As discussed above, the electric field \( \mathbf{E} \) on the \( \Gamma_{\text{PEC}} \) fades away. In the TM\(_z\) mode (2.1.20), \( E_z \), thus, located on the PEC wall remains zero. To further derive extra boundary conditions on PEC, we assume the interface \( \Gamma \) is vertical for simplicity. In this case, the normal direction coincides with the \( x \)-line, and then tangential direction will match the \( y \)-line, see Fig. 2.4. As a result, writing out the components of (2.6.3) for the simplest case of the TM\(_z\) mode, one gets the following relations holding for any point on the interface \( \Gamma \)

\[ E_y = 0, \quad E_z = 0, \quad H_x = 0. \tag{2.6.4} \]

Note that the value \( E_y \) is not needed in the TM\(_z\) mode, by taking the tangential derivative,
i.e. $y$ derivative, of (2.6.4), we arrive at

$$\frac{\partial E_z}{\partial y} = 0, \quad \frac{\partial H_x}{\partial y} = 0, \quad \text{on } \Gamma_{\text{PEC}}. \quad (2.6.5)$$

By realizing that $\frac{\partial E_z}{\partial t} = 0$ and using (2.6.5), the last equation in system (2.5.7) gives us

$$\frac{\partial H_y}{\partial x} = 0, \quad \text{on } \Gamma_{\text{PEC}}. \quad (2.6.6)$$

Taking time derivative of the last equation in system (2.5.7), one attains

$$0 = \frac{\partial^2 E_z}{\partial t^2} = \frac{1}{\mu} \left( \frac{\partial^2 E_z}{\partial y^2} + \frac{\partial^2 E_z}{\partial x^2} \right), \quad \text{on } \Gamma_{\text{PEC}}. \quad (2.6.7)$$

Combining (2.6.5) and (2.6.7) to deduce $\frac{\partial^2 E_z}{\partial x^2} = 0$ on the PEC wall. At this stage, the boundary conditions on PEC are explicitly given by

$$E_z = 0, \quad \frac{\partial^2 E_z}{\partial x^2} = 0, \quad \frac{\partial^2 E_z}{\partial y^2} = 0, \quad \frac{\partial H_x}{\partial y} = 0, \quad \frac{\partial H_y}{\partial x} = 0. \quad (2.6.8)$$

We note that the boundary conditions (2.6.8) allow us to have an anti-symmetric boundary extension on $E_z$, and symmetric boundary extensions on $H_x$ and $H_y$ [46]. Consequently, these boundary conditions can be effectively used for high-order finite-difference methods.

### 2.7 The perfectly matched layer

One of the greatest challenges in the computational electromagnetics (CEM) is how to provide an effective and accurate approach to deal with the wave interaction problems in unbounded domains. In the practical use of the finite-difference methods, the computational regions have to be truncated to save the memory resources. That object gives rise to the development of the absorbing boundary conditions (ABC) which are employed to terminate the incoming waves. There is a number of analytical techniques introduced to accomplish that aim [47–50]. However these techniques only work under certain circumstances. Indeed,
these analytical ABCs is function of the incident angle which results in a high reflective coefficient for the grazing angle [38].

In 1994, the aforementioned difficulty is overcome by Berenger. In his paper [51], Berenger proposed a novel approach named the perfectly matched layer (PML) which will be insightfully discussed in Chapter 7. The advance in the PML is to absorb the incident waves with arbitrary angle and frequency by constructing matched parameters at the boundary. In the simulations, PML is placed around the interested domain to terminate the reflected from this area, and the outer region is enforced by PEC as the boundary conditions, see Fig. 2.5.

Since the Berenger’s first paper, a different idea using a stretched-coordinate form introduced by Chew and Weedon in the same year 1994 [52]. A new efficient implementation for this approach was proposed by Roden and Gedney in [53] based on a recursive-convolution technique. Therefore, it has been refered to as the CPML formulation, and is arguably the best PML approach today.
In this section, we will discuss briefly the stretched-coordinate formulation developed by Chew and Weedon in [52]. In the PML, a modified Maxwell’s equations is given in the frequency domain as follows

\[ \nabla_e \times \mathbf{E} = j\omega \mu_2 \mathbf{H}, \quad (2.7.1) \]
\[ \nabla_h \times \mathbf{H} = -j\omega \varepsilon \mathbf{E}, \quad (2.7.2) \]

with

\[ \nabla_e = \hat{x} \frac{1}{e_x} \frac{\partial}{\partial x} + \hat{y} \frac{1}{e_y} \frac{\partial}{\partial y} + \hat{z} \frac{1}{e_z} \frac{\partial}{\partial z}, \quad (2.7.3) \]
\[ \nabla_h = \hat{x} \frac{1}{h_x} \frac{\partial}{\partial x} + \hat{y} \frac{1}{h_y} \frac{\partial}{\partial y} + \hat{z} \frac{1}{h_z} \frac{\partial}{\partial z}, \quad (2.7.4) \]

where \( e_i, h_i \) (\( i = x, y, z \)) are the complex stretching variables and will be determined in the matching conditions to eliminate the reflected waves at the boundary, see Fig. 2.6.

At the perfectly matched interface, by following the interface condition (2.6.1), one gets...
the following matching conditions \[ 52 \]

\[
\epsilon_2 = \epsilon_1, \quad \mu_2 = \mu_1, \quad (2.7.5)
\]

\[
e_x = h_x = s_x \in \mathbb{C}, \quad e_y = h_y = s_y \in \mathbb{C}, \quad e_z = h_z = s_z \in \mathbb{C}. \quad (2.7.6)
\]

To reduce the reflection coefficient at low frequencies, the tensor coefficients \( s_w \) (\( w = x, y \) and \( z \)) are chosen as follows \[ 43 \]

\[
s_w = \kappa_w + \frac{\sigma_w}{a_w + j\omega\epsilon_0}, \quad (2.7.7)
\]

where

\[
\sigma_w(w) = \left(\frac{w}{d}\right)^m \sigma_{x,\text{max}}, \quad (2.7.8)
\]

\[
\kappa_w(w) = 1 + (\kappa_{w,\text{max}} - 1) \left(\frac{w}{d}\right)^m, \quad (2.7.9)
\]

\[
a_w(w) = \left(\frac{d - x}{d}\right)^{m_a}, \quad (2.7.10)
\]

In the above, we consider the polynomial grading for the parameters, and \( d \) is the PML thickness. For the optimal result, powers \( m \) and \( m_a \) can be chosen as 2 or 3 \[ 43 \].

The stretched coordinate form of the PML for the 3D Maxwell’s equations is, then, expressed in the time-domain as

\[
\frac{\partial \mathbf{D}}{\partial t} = \mathbf{x} \left( \tilde{s}_y \ast \frac{\partial H_z}{\partial y} - \tilde{s}_z \ast \frac{\partial H_y}{\partial z} \right) + \mathbf{y} \left( \tilde{s}_z \ast \frac{\partial E_x}{\partial z} - \tilde{s}_x \ast \frac{\partial E_z}{\partial x} \right) + \mathbf{z} \left( \tilde{s}_x \ast \frac{\partial H_y}{\partial x} - \tilde{s}_y \ast \frac{\partial H_x}{\partial y} \right), \quad (2.7.11)
\]

\[
-\frac{\partial \mathbf{B}}{\partial t} = \mathbf{x} \left( \tilde{s}_y \ast \frac{\partial E_z}{\partial y} - \tilde{s}_z \ast \frac{\partial E_y}{\partial z} \right) + \mathbf{y} \left( \tilde{s}_z \ast \frac{\partial E_x}{\partial z} - \tilde{s}_x \ast \frac{\partial E_z}{\partial x} \right) + \mathbf{z} \left( \tilde{s}_x \ast \frac{\partial E_y}{\partial x} - \tilde{s}_y \ast \frac{\partial E_x}{\partial y} \right), \quad (2.7.12)
\]
where $\star$ denotes a convolution, and $\tilde{s}_w$ ($w = x, y$ and $z$) is defined by

$$
\tilde{s}_w = \mathcal{F}^{-1}\left(\frac{1}{s_w}\right),
$$

in which $\mathcal{F}^{-1}$ denote the inverse Fourier transform.

Since the stretched-coordinate formulation does not use the split-field PML as Berenger’s approach, it allows us to conveniently formulate the PML with different types of structure without splitting the field components at the beginning of the computation. In addition, the PML formulation mentioned in (2.7.11) and (2.7.12) has nothing to do with the constitutive relations, therefore it can be easily extended to arbitrary and nonlinear materials.
Chapter 3

TIME-DOMAIN MATCHED INTERFACE AND BOUNDARY METHODS FOR DIELECTRIC INTERFACE PROBLEMS

This chapter is based on our published work [54].

3.1 Introduction

A Dielectric material is considered as an electric insulator but an effective supporter of electrostatic fields. When a dielectric plate is placed in the electric field, it will prevent the electric charges from going through the material and causes the dielectric polarization. As a result, the dielectric materials can be used to increase the capacitance by reducing the electric field strength. Dielectrics are very important in the study of optical devices, microwave circuits, antennas, aircraft radar signature, nano/micro electric devices, and telecommunication chips. All those areas concern the interface problems.

In the dielectric interface problem, a dielectric interface $\Gamma$ separates a domain $\Omega$ in two parts $\Omega^-$ and $\Omega^+$ as shown in Fig. 3.1. For simplicity, the domain $\Omega$ is assumed to be a rectangle one $\Omega = [a, b] \times [c, d]$, with proper boundary conditions prescribed for $u$ on $\partial \Omega$. Across a material interface $\Gamma$, material coefficients $\epsilon$ and $\mu$ could be discontinuous. We define the jump of a function $u(x, y)$ at $\Gamma$ to be $[u] := u^+ - u^-$. The superscript, $-$ or $+$, denotes the limiting value of function from inside or outside of the interface. Without the loss of generality, the subdomain $\Omega^+$ is assumed to be the air or vacuum with $\epsilon^+ = \mu^+ = 1$, whereas the inside subdomain $\Omega^-$ is assigned to be a dielectric medium.

For convenience, let us recall the 2D Maxwell’s equations including TM$_z$ and TE$_z$ modes
Figure 3.1: A dielectric interface $\Omega$ separating two media over the domain.

for the nondispersive materials already derived at (2.5.7) and (2.5.8)

\[
\begin{align*}
\text{TM}_z \text{ mode :} & \quad \frac{\partial E_z}{\partial t} = \frac{1}{\epsilon} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right), \quad \frac{\partial H_y}{\partial t} = \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \quad \frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \frac{\partial E_z}{\partial y}, \\
\text{TE}_z \text{ mode :} & \quad \frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right), \quad \frac{\partial E_y}{\partial t} = -\frac{1}{\epsilon} \frac{\partial H_z}{\partial x}, \quad \frac{\partial E_x}{\partial t} = \frac{1}{\epsilon} \frac{\partial H_z}{\partial y},
\end{align*}
\]

Across the material interface, based on (2.6.1), the field solutions on both media are physically related through the jump conditions as

\[
\begin{align*}
\vec{n} \times (E^+ - E^-) &= 0, \quad \vec{n} \cdot (\epsilon^+ E^+ - \epsilon^- E^-) = 0, \\
\vec{n} \times (H^+ - H^-) &= 0, \quad \vec{n} \cdot (\mu^+ H^+ - \mu^- H^-) = 0,
\end{align*}
\]

where $\vec{n}$ is the unit normal vector to the interface, pointing from $\Omega^-$ to $\Omega^+$. These zeroth order jump conditions suggest that the tangential components of $E$ and $H$ are continuous, while their normal components could be discontinuous. Combining the zeroth order jump conditions (3.1.3) with Maxwell’s equations (3.1.1) and (3.1.2), we can derive first order jump conditions describing the regularities in the first derivatives of $E$ and $H$ [26, 34]. Higher order jump conditions can be derived in a similar manner, but become very complicated so that
they are usually skipped in the numerical interface treatments [26].

As expected, when the permittivity and permeability coefficients are discontinuous across a material interface separating two dielectric media, the electric and magnetic field components could be discontinuous. Without a proper interface treatment, the time domain numerical solution of Maxwell’s equations that govern the propagation and scattering of electromagnetic waves in nonhomogeneous media converges slowly or even fails to converge [25]. Consequently, the classical approach, i.e. the Yee scheme in Section 2.5 only achieves first-order accuracy in the interface problems [7–9]. Therefore, the development of innovative computational methods for dealing with electromagnetic interface problems with discontinuous solutions has received much attention in recent years. Various different embedded FDTD methods have been developed in the computational electromagnetics (CEM) to cope with the problems caused by the loss of solution regularity and the complex geometry of the material interface [25, 27–33]. In this work, we will present a novel FDTD method to successfully restore the second-order accuracy of the curved dielectric-interface problems.

3.2 Matched Interface and boundary (MIB) algorithm

In this section, we propose a novel MIB time-domain (MIBTD) algorithm for solving the discontinuous Maxwell interface problem. Previously, several MIBTD schemes were developed for solving regular dielectric interface problems [26, 34]. However, the electromagnetic fields are assumed to be continuous across the interface in these existing studies. We note that for the scalar elliptic and parabolic interface problems, robust MIB schemes [55, 56] have been constructed to handle discontinuous solutions. Nevertheless, these discontinuous interface treatments can not be directly applied to the present Maxwell interface problem, which is of a vectorial nature, i.e., different field components will be coupled through the jump conditions. Moreover, in the Yee mesh, the field components are located in staggered positions. This introduces additional difficulties for solving Maxwell interface problems.
3.2.1 Finite difference Time domain (FDTD) discretization based on MIB

Without the loss of generality, we will present the new MIBTD algorithm by considering the TM system (3.1.1). The MIBTD method for solving the TE system (3.1.2) can be similarly constructed.

Denote the time increment to be $\Delta t$. Both electric and magnetic components will be assumed at the same time instant $t_k = k\Delta t$ in the MIBTD algorithm. The classical fourth order Runge-Kutta scheme will be employed to integrate the TM system (3.1.1) from $t_k$ to $t_{k+1}$. A uniform staggered grid shown in Fig. 2.1 is used in the MIBTD algorithm. Denote $\Delta x$ and $\Delta y$ to be the spacing in $x$ and $y$ direction, respectively. To facilitate the following discussions, we adopt the following notations: $E_{z,i,j} := E_z(x_i, y_j, t_k)$, $H_{x,i,j+\frac{1}{2}} := H_x(x_i, y_{j+\frac{1}{2}}, t_k)$, and $H_{y,i+\frac{1}{2},j} := H_y(x_{i+\frac{1}{2}}, y_j, t_k)$. For nodes away from the interface, the central finite difference approximations as in the standard FDTD algorithm are employed for the spatial discretization, e.g.,

$$\frac{\partial H_y}{\partial x} \bigg|_{(x_i, y_j)} \approx \frac{H_{y,i+\frac{1}{2},j} - H_{y,i-\frac{1}{2},j}}{\Delta x}. \quad (3.2.1)$$

For nodes near $\Gamma$, the MIB interface treatment [26, 55] will be carried out to correct finite difference approximations via rigorously imposing the jump conditions. A universal rule here is that to approximate function or its derivatives on one side of interface, one never directly refers to function values from the other side. Instead, fictitious values form the other side of the interface will be supplied. For example, suppose that $\Gamma$ cuts the grid line $y = y_j$ in between $x_i$ and $x_{i+\frac{1}{2}}$. We need to determine a fictitious value of $H_y$ at $(x_{i+\frac{1}{2}}, y_j)$. We denote it as $f_{y,i+\frac{1}{2},j}$. Then the approximation (3.2.1) shall be modified to be

$$\frac{\partial H_y}{\partial x} \bigg|_{(x_i, y_j)} \approx \frac{f_{y,i+\frac{1}{2},j} - H_{y,i-\frac{1}{2},j}}{\Delta x}. \quad (3.2.2)$$
Likewise, if $\Gamma$ passes the line $y = y_j$ in between $x_{i-\frac{1}{2}}$ and $x_i$, (3.2.1) will be changed to

$$\frac{\partial H_y}{\partial x} \bigg|_{(x_i,y_j)} \approx \frac{H^y_{i+\frac{1}{2},j} - f^y_{i-\frac{1}{2},j}}{\Delta x}. \quad (3.2.3)$$

These corrected approximations maintain the second order of accuracy, provided that fictitious values are accurately estimated by using the jump conditions (3.1.3).

### 3.2.2 Interface jump conditions in a local coordinate

Since jump conditions (3.1.3) are physically defined in terms of normal and tangential directions, we first derive jump conditions in a local coordinate. Consider a point $P(x_o,y_o)$ located on the interface $\Gamma$. We define a local coordinate system $(\vec{n},\vec{\tau})$ at $P$, see Fig. 3.2. Any nearby point $(x,y)$ will have local coordinate values

$$n = \cos \theta x + \sin \theta y, \quad \tau = -\sin \theta x + \cos \theta y, \quad (3.2.4)$$

where $0 \leq \theta < 2\pi$ is the angle between the positive $x$-direction and the normal vector $\vec{n}$ at $P$. It is also worthwhile mentioning the derivative operators on this local coordinate

$$\frac{\partial}{\partial n} = \cos \theta \frac{\partial}{\partial x} + \sin \theta \frac{\partial}{\partial y}, \quad \frac{\partial}{\partial \tau} = -\sin \theta \frac{\partial}{\partial x} + \cos \theta \frac{\partial}{\partial y}. \quad (3.2.5)$$

On the local grid system, jump conditions (3.1.3) give us the following zeroth order jump conditions

$$[E_z] = 0, \quad [E_\tau] = 0, \quad [\epsilon E_n] = 0, \quad [H_z] = 0, \quad [H_\tau] = 0, \quad [\mu H_n] = 0. \quad (3.2.6)$$

First order jump conditions of all fields can be implied based on the zeroth order conditions (3.2.6) and Maxwell’s equations [7, 8, 26]. For the $E_z$ component, one jump condition can be derived by taking the derivative with respect to the tangent direction of the first equation
Figure 3.2: Local normal and tangential coordinate of a point on the interface $\Gamma$.

in (3.2.6)

$$
\left[ \frac{\partial E_z}{\partial \tau} \right] = 0.
$$

(3.2.7)

To seek for another jump condition of this field, we rewrite the second equation of (3.1.1) in

local coordinate and then apply the jump operators on it to obtain

$$
\left[ \frac{1}{\mu} \frac{\partial E_z}{\partial n} \right] = \left[ \frac{\partial H_\tau}{\partial t} \right] = 0,
$$

(3.2.8)

where we make use of the fact $[H_\tau] = 0$. Concerning the jump conditions of the magnetic

component, one takes the derivative with respect to $\tau$ of the two last conditions in (3.2.6)

to achieve

$$
\left[ \frac{\partial H_\tau}{\partial \tau} \right] = 0, \quad \left[ \frac{\partial (\mu H_n)}{\partial \tau} \right] = 0.
$$

(3.2.9)

Another jump condition of magnetic field can be derived by employing the divergence free

law

$$
\nabla \cdot (\mu H) = \frac{\partial (\mu H_n)}{\partial n} + \frac{\partial (\mu H_\tau)}{\partial \tau} + \frac{\partial (\mu H_z)}{\partial z} = 0,
$$

(3.2.10)

In the TM mode, all of the fields are uniform along the $z$-direction. Therefore, their deriva-
tives with respect to $z$ can be omitted. Consequently, equation (3.2.10) becomes in a simpler
form

\[
\frac{\partial (\mu H_n)}{\partial n} + \frac{\partial (\mu H_\tau)}{\partial \tau} = 0,
\]  

(3.2.11)

We take jump values on both hand sides of equation (3.2.11)

\[
\left[\frac{\partial (\mu H_\tau)}{\partial \tau}\right] + \left[\frac{\partial (\mu H_n)}{\partial n}\right] = 0.
\]  

(3.2.12)

One multiplies the first equation of (3.1.1) by \(\mu\) and then takes jump operators on it to give rise to the last jump condition of \(H\) field

\[
\left[\frac{\partial (\mu H_\tau)}{\partial n}\right] - \left[\frac{\partial (\mu H_n)}{\partial \tau}\right] = \left[\frac{\partial (\mu \epsilon E_z)}{\partial t}\right].
\]  

(3.2.13)

We note that the condition (3.2.13) is a new condition which has never been used in the previous MIBTD schemes. In its present form, (3.2.13) contains a time dependent part. Nevertheless, we will show later that this term can be estimated based on known \(H_x\) and \(H_y\) values at time \(t_k\).

### 3.2.3 Interface jump conditions in the Cartesian coordinate

Since all the FDTD spatial discretization is conducted in the Cartesian directions, we need to transform the jump conditions in the local coordinate into the Cartesian ones. Moreover, a key idea in the MIB interface treatment is to decompose the 2D jump conditions so that they can be imposed in a 1D manner [34, 55]. We will consider such decompositions, while taking care of the coordinate transformations.

We first consider the zeroth order jump conditions for Cartesian field components. For \(E_z\), we simply have

\[
E_z^+ - E_z^- = 0.
\]  

(3.2.14)

In order to derive the jump conditions for \(H_x\) and \(H_y\), one can use coordinate transformation
mentioned in (3.2.4) to translate the zeroth order jump conditions \([H_r] = 0\) and \([\mu H_n] = 0\) into

\[
0 = [H_r] = -\sin \theta H^+_x + \cos \theta H^+_y + \sin \theta H^-_x - \cos \theta H^-_y, \tag{3.2.15}
\]

\[
0 = [\mu H_n] = \cos \theta \mu^+ H^+_x + \sin \theta \mu^+ H^+_y - \cos \theta \mu^- H^-_x - \sin \theta \mu^- H^-_y. \tag{3.2.16}
\]

Because our incident waves propagate from the positive side, \(H^-_x\) will be eliminated from (3.2.15) and (3.2.16) to obtain

\[
C^+_x H^+_x + C^+_y H^+_y - C^-_x H^-_y = 0, \tag{3.2.17}
\]

in which

\[
C^+_x = (\mu^+ - \mu^-) \cos \theta \sin \theta, \quad C^+_y = \sin^2 \theta \mu^+ + \cos^2 \theta \mu^-, \quad \text{and} \quad C^-_y = \mu^-.
\]

Similarly, the new jump condition will be derived by canceling \(H^-_y\) from (3.2.15) and (3.2.16)

\[
D^+_x H^+_x + D^+_y H^+_y - D^-_x H^-_x = 0, \tag{3.2.18}
\]

where

\[
D^+_x = \sin^2 \theta \mu^- + \cos^2 \theta \mu^+, \quad D^+_y = (\mu^+ - \mu^-) \sin \theta \cos \theta, \quad \text{and} \quad D^-_x = \mu^-.
\]

For seeking the first order jump conditions of all fields in the Cartesian grid, one can use first derivative operator in (3.2.5). Then the first order jump conditions of \(E_z\) component in

43
the Cartesian grid arise as follows

\[
0 = \left[ \frac{1}{\mu} \frac{\partial E_z}{\partial n} \right] = \cos \theta \frac{1}{\mu^+} \left( \frac{\partial E_z}{\partial x} \right)^+ + \sin \theta \frac{1}{\mu^+} \left( \frac{\partial E_z}{\partial y} \right)^+ - \cos \theta \frac{1}{\mu^-} \left( \frac{\partial E_z}{\partial x} \right)^- \\
- \sin \theta \frac{1}{\mu^-} \left( \frac{\partial E_z}{\partial y} \right)^- , \tag{3.2.19}
\]

\[
0 = \left[ \frac{\partial E_z}{\partial \tau} \right] = -\sin \theta \left( \frac{\partial E_z}{\partial x} \right)^+ + \cos \theta \left( \frac{\partial E_z}{\partial y} \right)^+ + \sin \theta \left( \frac{\partial E_z}{\partial x} \right)^- \\
- \cos \theta \left( \frac{\partial E_z}{\partial y} \right)^- . \tag{3.2.20}
\]

If the extrapolation is conducted from the positive side, one will cancel \((\partial E_z/\partial y)^-\) from (3.2.19) and (3.2.20) to achieve

\[
A_x^+ \left( \frac{\partial E_z}{\partial x} \right)^+ + A_y^+ \left( \frac{\partial E_z}{\partial y} \right)^+ - A_x^- \left( \frac{\partial E_z}{\partial x} \right)^- = 0, \tag{3.2.21}
\]

where

\[
A_x^+ = \frac{1}{\mu^+} \cos \theta + \frac{1}{\mu^-} \tan \theta \sin \theta, \quad A_y^+ = \frac{1}{\mu^+} \sin \theta - \frac{1}{\mu^-} \sin \theta, \quad A_x^- = \frac{1}{\mu^-} \cos \theta + \frac{1}{\mu^-} \tan \theta \sin \theta.
\]

Another first order jump condition for \(E_z\) shall be derived by canceling \((\partial E_z/\partial x)^-\) from (3.2.19) and (3.2.20)

\[
B_x^+ \left( \frac{\partial E_z}{\partial x} \right)^+ + B_y^+ \left( \frac{\partial E_z}{\partial y} \right)^+ - B_y^- \left( \frac{\partial E_z}{\partial y} \right)^- = 0, \tag{3.2.22}
\]

where

\[
B_x^+ = \left( \frac{1}{\mu^+} - \frac{1}{\mu^-} \right) \cos \theta, \quad B_y^+ = \frac{1}{\mu^-} \cos \theta \cot \theta + \frac{1}{\mu^+} \sin \theta
\]

and \(B_y^- = \frac{1}{\mu^-} (\cos \theta \cot \theta + \sin \theta)\).

We note that the zeroth jump condition (3.2.14) and two first order jump conditions (3.2.21)
and (3.2.22) for $E_z$ are in the standard form, as discussed in the classical MIB scheme [55]. It is clear to see that the above jump conditions are only valid when the normal direction is not aligned to $x-$ or $y-$ direction. Otherwise, jump conditions (3.2.21) and (3.2.22) will be simplified as

$$\frac{1}{\mu^+} \left( \frac{\partial E_z}{\partial x} \right)^+ - \frac{1}{\mu^-} \left( \frac{\partial E_z}{\partial x} \right)^- = 0. \quad (3.2.23)$$

Moreover, these conditions only involves $E_z$ field over integer grid nodes $(x_i, y_j)$ on the Yee lattice (see Fig. 2.1). Therefore, the MIB modeling of $E_z$ can be simply handled by the classical MIB scheme [55].

The situation for $H_x$ and $H_y$ becomes much more complicated. To attain the first order jump conditions for $H_x$ and $H_y$, we again employ the coordinate transformations defined in (3.2.4) and (3.2.5). For the condition (3.2.13), we have

$$\left[ \frac{\partial (\mu H_y)}{\partial x} \right] - \left[ \frac{\partial (\mu H_x)}{\partial y} \right] = \left[ \frac{\partial (\mu \epsilon E_z)}{\partial t} \right] = \left( \mu^+ \epsilon^+ - \mu^- \epsilon^- \right) \frac{\partial E_z}{\partial t}$$

$$= \frac{\mu^+ \epsilon^+ - \mu^- \epsilon^-}{\epsilon^+} \left\{ \left( \frac{\partial H_y}{\partial x} \right)^+ - \left( \frac{\partial H_x}{\partial y} \right)^+ \right\} \quad (3.2.24)$$

Here we have utilized the equation $[E_z] = 0$ and the TM Maxwell’s equations to simplify the right hand side. The non-homogeneous term indeed becomes time independent, as we
mentioned above. For conditions (3.2.9) and (3.2.12), we similarly have

\[ 0 = \left[ \frac{\partial (\mu H_n)}{\partial n} \right] + \left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right] = \left[ \frac{\partial (\mu H_x)}{\partial x} \right] + \left[ \frac{\partial (\mu H_y)}{\partial y} \right] \]  \quad (3.2.25)

\[ 0 = \left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right] = \sin^2 \theta \left[ \frac{\partial (\mu H_x)}{\partial x} \right] - \cos \theta \sin \theta \left[ \frac{\partial (\mu H_x)}{\partial y} \right] - \sin \theta \cos \theta \left[ \frac{\partial (\mu H_y)}{\partial x} \right] 
+ \cos^2 \theta \left[ \frac{\partial (\mu H_y)}{\partial y} \right], \]  \quad (3.2.26)

\[ 0 = \left[ \frac{\partial (\mu H_n)}{\partial \tau} \right] = -\sin \theta \cos \theta \left[ \frac{\partial (\mu H_x)}{\partial x} \right] + \cos^2 \theta \left[ \frac{\partial (\mu H_x)}{\partial y} \right] - \sin^2 \theta \left[ \frac{\partial (\mu H_y)}{\partial x} \right] 
+ \cos \theta \sin \theta \left[ \frac{\partial (\mu H_y)}{\partial y} \right]. \]  \quad (3.2.27)

By solving four equations (3.2.24), (3.2.25), (3.2.26) and (3.2.27), we attain four simplified jump conditions

\[ \left[ \frac{\partial (\mu H_y)}{\partial x} \right] = \cos^2 \theta C_0 \left\{ \left( \frac{\partial H_y}{\partial x} \right)^+ - \left( \frac{\partial H_x}{\partial y} \right)^+ \right\} - \sin(2\theta) \left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right], \]  \quad (3.2.28)

\[ \left[ \frac{\partial (\mu H_x)}{\partial x} \right] = -\frac{\sin(2\theta)}{2} C_0 \left\{ \left( \frac{\partial H_y}{\partial x} \right)^+ - \left( \frac{\partial H_x}{\partial y} \right)^+ \right\} - \cos(2\theta) \left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right], \]  \quad (3.2.29)

\[ \left[ \frac{\partial (\mu H_y)}{\partial y} \right] = \frac{\sin(2\theta)}{2} C_0 \left\{ \left( \frac{\partial H_y}{\partial x} \right)^+ - \left( \frac{\partial H_x}{\partial y} \right)^+ \right\} + \cos(2\theta) \left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right], \]  \quad (3.2.30)

\[ \left[ \frac{\partial (\mu H_x)}{\partial y} \right] = -\sin^2 \theta C_0 \left\{ \left( \frac{\partial H_y}{\partial x} \right)^+ - \left( \frac{\partial H_x}{\partial y} \right)^+ \right\} - \sin(2\theta) \left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right], \]  \quad (3.2.31)

where

\[ C_0 = \frac{\mu^+ \epsilon^+ - \mu^- \epsilon^-}{\epsilon^+}. \]
Now note that term \( \partial (\mu H_\tau) / \partial \tau \) remains unknown, but can be further simplified as follows

\[
\left[ \frac{\partial (\mu H_\tau)}{\partial \tau} \right] = (\mu^+ - \mu^-) \left( \frac{\partial H_\tau}{\partial \tau} \right)^+ + \mu^- \left[ \frac{\partial H_\tau}{\partial \tau} \right] \\
= (\mu^+ - \mu^-) \left[ \sin^2 \theta \left( \frac{\partial H_x}{\partial x} \right)^+ - \cos \theta \sin \theta \left( \frac{\partial H_x}{\partial y} \right)^+ - \sin \theta \cos \theta \left( \frac{\partial H_y}{\partial x} \right)^+ \\
+ \cos^2 \theta \left( \frac{\partial H_y}{\partial y} \right)^+ \right],
\]

(3.2.32)

Note that \( \left[ \frac{\partial H_\tau}{\partial \tau} \right] = 0 \). So it is dropped out in the derivation. Since \( \mu \) is a piecewise constant across the interface, Eq. (3.2.11) can be deduced to another equation

\[
\frac{\partial H_x}{\partial x} = -\frac{\partial H_y}{\partial y}, 
\]

(3.2.33)

for either positive or negative side, but not the both sides. One combines (3.2.28),(3.2.32) and (3.2.33) to achieve

\[
C_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + C_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ + C_{yy}^+ \left( \frac{\partial H_y}{\partial y} \right)^+ = C_{yx}^- \left( \frac{\partial H_y}{\partial x} \right)^-, 
\]

(3.2.34)

where

\[
C_{xy}^+ = -\frac{\sin^2(2\theta)}{2}(\mu^+ - \mu^-) + \cos^2 \theta C_0, \quad C_{yx}^+ = \mu^+ - \frac{\sin^2(2\theta)}{2}(\mu^+ - \mu^-) - \cos^2 \theta C_0, \\
C_{yy}^+ = \frac{\sin(4\theta)}{2} \theta (\mu^+ - \mu^-), \quad \text{and} \quad C_{yx}^- = \mu^-.
\]

Similarly, we also get the following jump conditions for magnetic components

\[
D_{xx}^+ \left( \frac{\partial H_x}{\partial x} \right)^+ + D_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + D_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ = D_{xx}^- \left( \frac{\partial H_x}{\partial x} \right)^-, 
\]

(3.2.35)

\[
\hat{C}_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + \hat{C}_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ + \hat{C}_{yy}^+ \left( \frac{\partial H_y}{\partial y} \right)^+ = \hat{C}_{yx}^- \left( \frac{\partial H_y}{\partial x} \right)^-, 
\]

(3.2.36)

\[
\hat{D}_{xx}^+ \left( \frac{\partial H_x}{\partial x} \right)^+ + \hat{D}_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + \hat{D}_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ = \hat{D}_{xy}^- \left( \frac{\partial H_x}{\partial y} \right)^-, 
\]

(3.2.37)
where

\[
D_{xx}^+ = \mu^+ - \cos^2(2\theta)(\mu^+ - \mu^-),\quad D_{xy}^+ = -\frac{\sin(4\theta)}{4}(\mu^+ - \mu^-) - \frac{\sin(2\theta)C_0}{2},
\]
\[
D_{yx}^+ = -\frac{\sin(4\theta)}{4}(\mu^+ - \mu^-) + \frac{\sin(2\theta)C_0}{2},
\]
\[
D_{xx}^- = \mu^-,
\]
\[
\hat{C}_{xy}^+ = \frac{\sin(4\theta)}{4}(\mu^+ - \mu^-) + \frac{\sin(2\theta)C_0}{2},\quad \hat{C}_{yx}^+ = \frac{\sin(4\theta)}{4}(\mu^+ - \mu^-) - \frac{\sin(2\theta)C_0}{2},
\]
\[
\hat{C}_{yy}^+ = \mu^+ - \cos^2(2\theta)(\mu^+ - \mu^-),\quad \hat{C}_{yy}^- = \mu^-,
\]
\[
\hat{D}_{xx}^+ = -\frac{\sin(4\theta)}{2}(\mu^+ - \mu^-),\quad \hat{D}_{xy}^+ = \mu^+ - \frac{\sin^2(2\theta)}{2}(\mu^+ - \mu^-) - \sin^2 \theta C_0,
\]
\[
\hat{D}_{yx}^+ = -\frac{\sin^2(2\theta)}{2}(\mu^+ - \mu^-) + \sin \theta C_0,\quad \hat{D}_{xy}^- = \mu^-,
\]
\[
\hat{D}_{yx}^- = \mu^- - \frac{\sin^2 \theta C_0}{\epsilon^+},\quad C_0 = \frac{\mu^+ \epsilon^+ - \mu^- \epsilon^-}{\epsilon^+}.
\]

We note that jump conditions for \(H_x\) and \(H_y\) are mixed together in these equations. This is a feature not seeing in scalar elliptic and parabolic interface problems \([55, 56]\). A novel MIB scheme has to be developed to address this issue. In the proposed MIB scheme for the TM equation, jump conditions \((3.2.17), (3.2.18), (3.2.34)\) and \((3.2.35)\) are used for correcting the derivatives of magnetic fields along the \(x\) direction, while jump conditions \((3.2.17), (3.2.18), (3.2.36)\) and \((3.2.37)\) are applied for seeking fictitious values of magnetic fields in the \(y\) direction. The jump conditions for the TE mode can be similarly derived.

### 3.2.4 Jump conditions implementation

In this subsection, we discuss how to implement the jump conditions derived above in the MIB scheme to determine the necessary fictitious values for the FDTD discretization. To save the space, only MIB treatment for the TM mode is illustrated here. For the \(E_z\) component of the TM mode, the jump conditions are standard, so that the classical MIB scheme \([55]\) can be simply applied. A new MIB scheme is proposed to treat \(H_x\) and \(H_y\) in this subsection.

The essence of the MIB scheme is to impose jump conditions in a 1D manner. Thus, the MIB treatments in \(x\) and \(y\) directions are essentially the same. It is sufficient to discuss the
Figure 3.3: Illustration of the MIB grid partition. Filled circles: grid nodes for $H_y$; Fill triangles: nodes for $H_x$; Open circles: fictitious nodes for $H_y$; Open triangle: fictitious nodes for $H_x$; Open squares: auxiliary nodes for $H_y$ and $H_x$; Square: interface node $(x_o, y_o)$.

MIB treatment of $H_x$ and $H_y$ along the $x$ direction in the present study. The modeling along the $y$ direction can be similarly carried out. For the $x$ direction, a group of jump conditions including Eqs. (3.2.17), (3.2.18), (3.2.34) and (3.2.35), will be studied. As in other Cartesian grid methods, in the MIB scheme, grid points are classified as irregular grid points if the standard finite approximation refers to a node from the other side of the interface. Otherwise they will be classified as regular grid points. For every irregular point, a fictitious value needs to be calculated through enforcing jump conditions.

A particular local grid topology is shown in Fig. 3.3. Here, we consider an interface point $(x_o, y_o)$ on the interface $\Gamma$. In the vicinity of $(x_o, y_o)$, the nodes $(x_{i-1/2}, y_j)$ and $(x_{i+1/2}, y_j)$ are the irregular grid points for $H_y$. We suppose that both $(x_{i-1/2}, y_j)$ and $(x_{i}, y_j)$ belong to $\Omega^-$ and $(x_{i+1/2}, y_j)$ belongs to $\Omega^+$. See Fig. 3.3. Following the notation defined above, we demonstrate how to determine four fictitious values $f_{i-1/2,j}^y$, $f_{i+1/2,j}^y$, $f_{i,j}^x$ and $f_{i+1,j}^x$ for the...
derivative approximation (l-subdomains. Here the subscript

\[ D \]

where \( C \) represents the interpolation \((l = 0)\) and the first order derivative approximation \((l = 1)\), and \( k \) is for grid index. The finite difference weights \( w_{l,k}^{-} \) and \( w_{l,k}^{+} \) are for \( H_y \), while the weights \( w_{l,k}^{-} \) and \( w_{l,k}^{+} \) are for \( H_x \), since \( H_x \) and \( H_y \) are on different locations in the Yee mesh.

Only \( x \) derivatives are discretized in Eqs. \((3.2.38) - (3.2.41)\), whereas three \( y \) derivatives at the interface point \((x_o, y_o)\) remain unsolved. In order to approximate \((\partial H_y/\partial y)^+\) at \((x_o, y_o)\),
we introduce three auxiliary points \((x_o, y_o), (x_o, y_{j+1})\) and \((x_o, y_{j+2})\) on the positive side

\[
\left( \frac{\partial H_y}{\partial y} \right)_{x_o,y_o}^+ \approx p_{1,j}^+ \left( H_{o,j}^y \right)^+ + p_{1,j}^+ H_{o,j+1}^y + p_{1,j+2}^+ H_{o,j+2}^y. \tag{3.2.42}
\]

We note that \((H_{o,j}^y)^+\), \(H_{o,j+1}^y\) and \(H_{o,j+2}^y\) are evaluated on non-grid nodes. Therefore, they should be calculated by further interpolations. The grid nodes \((x_{i-1/2}, y_{j+1}), (x_{i+1/2}, y_{j+1}), (x_{i+3/2}, y_{j+1})\) and \((x_{i-3/2}, y_{j+2}), (x_{i-1/2}, y_{j+2}), (x_{i+1/2}, y_{j+2})\) are chosen to approximate \(H_{o,j+1}^y\) and \(H_{o,j+2}^y\) respectively. See Fig. 3.3. For evaluating \((H_{o,j}^y)^+\), one can refer it to the related grid nodes by using the following equation

\[
(H_{o,j}^y)^+ = \frac{C_x^+}{C_y^+} (H_{o,j}^x)^+ + \frac{C_y^-}{C_y^+} (H_{o,j}^y)^- \\
= -\frac{C_x^+}{C_y^+} \left( \bar{w}_{0,i}^+ f_{i,j}^x + \bar{w}_{0,j}^+ H_{i+1,j}^x + \bar{w}_{0,i+2}^+ H_{i+2,j}^x \right) \\
+ \frac{C_y^-}{C_y^+} \left( w_{0,i-\frac{1}{2}}^+ H_{i-\frac{1}{2},j}^y + w_{0,i-\frac{1}{2}}^- H_{i-\frac{1}{2},j}^y + w_{0,i+\frac{1}{2}}^- f_{i-\frac{1}{2},j}^y \right). \tag{3.2.43}
\]

Since \((\partial H_x/\partial y)^+\) is evaluated on the interface point \((x_o, y_o)\), it can be discretized in the same manner as the approximation of \((\partial H_y/\partial y)^+\)

\[
\left( \frac{\partial H_x}{\partial y} \right)_{x_o,y_o}^+ = \tilde{p}_{1,j}^+ \left( H_{o,j}^x \right)^+ + \tilde{p}_{1,j+\frac{1}{2}}^+ H_{o,j+\frac{1}{2}}^x + \tilde{p}_{1,j+\frac{3}{2}}^+ H_{o,j+\frac{3}{2}}^x. \tag{3.2.44}
\]

Similarly, grid nodes \((x_i, y_{j+1/2}), (x_{i+1}, y_{j+1/2}), (x_{i+2}, y_{j+1/2})\) and \((x_{i-1}, y_{j+3/2}), (x_{i}, y_{j+3/2}), (x_{i+1}, y_{j+3/2})\) are chosen to interpolate \(H_{o,j+1/2}^x\) and \(H_{o,j+3/2}^x\), respectively. See Fig. 3.3. Discretization of \((H_{o,j}^x)^+\) is achieved by adopting the following relation

\[
(H_{o,j}^x)^+ = -\frac{D_y^+}{D_x^+} H_y^+ + \frac{D_x^-}{D_x^+} H_x^- \\
= -\frac{D_y^+}{D_x^+} \left( w_{0,i-\frac{1}{2}}^+ f_{i-\frac{1}{2},j}^y + w_{0,i+\frac{1}{2}}^+ H_{i+\frac{1}{2},j}^y + w_{0,i+\frac{3}{2}}^- H_{i+\frac{3}{2},j}^y \right) \\
+ \frac{D_y^-}{D_x^+} \left( \bar{w}_{0,i-1}^+ H_{i-1,j}^x + \bar{w}_{0,i}^- H_{i,j}^x + \bar{w}_{0,i+1} f_{i+1,j}^x \right). \tag{3.2.45}
\]
By combining equations from (3.2.38) to (3.2.45) together, we obtain a system of equations which can be equivalently transferred into the following matrix form

\[ \mathbf{W} \cdot \mathbf{F} = \mathbf{C} \cdot \mathbf{U}, \quad (3.2.46) \]

where

\[
\mathbf{W} = [\mathbf{w}_1, \mathbf{w}_2, \mathbf{w}_3, \mathbf{w}_4]^\top \in \mathbb{R}^{4 \times 4}, \quad \mathbf{F} = \left[ f_i^{y_{i-1}}, f_i^{y_{i+1}}, f_i^{x_{i,j}}, f_i^{x_{i+1,j}} \right]^\top \in \mathbb{R}^{4 \times 1},
\]

\[
\mathbf{C} = [\mathbf{c}_1, \mathbf{c}_2, \mathbf{c}_3, \mathbf{c}_4]^\top \in \mathbb{R}^{4 \times 12}, \text{ and}
\]

\[
\mathbf{U} = \left[ H_i^{y_{i-1}}, H_i^{y_{i+1}}, H_i^{x_{i,j}}, H_i^{x_{i+1,j}}, H_{i,j+1}^{y_{i}}, H_{i,j+1}^{y_{i+1}}, H_{i,j+1}^{x_{i,j}}, H_{i,j+1}^{x_{i,j+1}}, H_{o,j+1}^{y_{i}}, H_{o,j+1}^{y_{i+1}}, H_{o,j+1}^{x_{i,j}}, H_{o,j+1}^{x_{i,j+1}} \right]^\top \in \mathbb{R}^{12 \times 1},
\]

where vectors

\[
\mathbf{w}_1^\top = \left( C_y^+ w_{0,i-\frac{1}{2}}, C_y^- w_{0,i+\frac{1}{2}}, -C_x^+ \bar{w}_{0,i}, 0 \right), \quad \mathbf{w}_2^\top = \left( -D_y^+ \bar{w}_{0,i-\frac{1}{2}}, D_x^- \bar{w}_{0,i+\frac{1}{2}} \right),
\]

\[
\mathbf{w}_3^\top = \left( -C_{x,y}^+ w_{1,i-\frac{1}{2}}^+, D_x^+ C_{x,y}^+ p_{1,j}^+, w_{0,i+\frac{1}{2}}^- , C_{x,y}^- w_{1,i+\frac{1}{2}}^- , -C_{y}^+ p_{1,j}^+ C_y^- w_{0,i+\frac{1}{2}}^- , -C_{x,x}^+ \bar{w}_{1,i} , C_y^+ C_{x,y}^+ p_{1,j}^+ \bar{w}_{0,i} , -C_{x,y}^+ \bar{p}_{1,j}^- D_x^- \bar{w}_{0,i+1} \right),
\]

\[
\mathbf{w}_4^\top = \left( -D_{x,y}^+ w_{1,i-\frac{1}{2}}^+, D_{x,y}^+ p_{1,j}^+ D_x^- w_{0,i}^+, -D_{y}^+ p_{1,j}^+ C_y^- w_{0,i+\frac{1}{2}}^- , -D_x^+ \bar{w}_{1,i}^+ , -D_{y}^+ p_{1,j}^+ C_y^+ \bar{w}_{0,i}^- , D_{x}^+ \bar{p}_{1,j}^- D_x^- \bar{w}_{0,i+1}^- \right),
\]
Then the fictitious values $\mathbf{F}$ are determined as the follows

$$
\mathbf{F} = \mathbf{W}^{-1} \cdot \mathbf{C} \cdot \mathbf{U}.
$$

(3.2.47)

Formulation (3.2.47) shows that fictitious values $\mathbf{F} = [f_{i-1/2,j}, f_{i+1/2,j}; f_{i+1,j}, f_{i+1,j+1}^x]^T$ are linear combinations of the function values in $\mathbf{U}$. In other words, they are determined by using 12 nearby $H_x$ and $H_y$ values. It is noted that the coefficients of fictitious values, i.e. $\mathbf{W}^{-1} \cdot \mathbf{C}$, only need to be generated once at the beginning. Then they can be re-used in all the subsequent time steps [26].

### 3.3 Experimental results

In this section, we examine the performance of the MIBTD method for solving discontinuous Maxwell interface problems. The stability, accuracy, and convergence of two algorithms will be investigated, by considering circular interface problems in both TM and TE modes. For simplicity, a square domain $\Omega = [-1, 1] \times [-1, 1]$ is used in all tests. Analytical solutions
are available to exactly verify numerical errors. For simplicity, the exact solutions will also be utilized for generating the initial solutions and boundary conditions in our computations. For convenience, the initial time and stopping time will be assigned to be \( t = 0 \) and \( t = T \) respectively. The time increment is denoted as \( \Delta t = T/N_t \), with \( N_t \) being the number of time steps.

In the MIBTD algorithm, a uniform Yee mesh is employed, in which the spacing in both \( x \) and \( y \) directions are the same, i.e., \( \Delta x = \Delta y \). For simplicity, we denote \( h = \Delta x = \Delta y \). Since \( \Omega \) is a square domain, the grid numbers in both \( x \) and \( y \) directions are also the same, and are denoted as \( N = N_x = N_y \) for the on-grid component, i.e., the \( E_z \) component in the TM mode and the \( H_z \) component in the TE mode. Denoting \( u_h(x_i, y_j, T) \) as the numerical approximation to a field component \( u(x, y, T) \) at time \( T \), we use the following measures to estimate \( L_\infty \) and \( L_2 \) errors of the MIBTD method

\[
L_\infty = \max_{i,j=1,...,N} |u(x_i, y_j, T) - u_h(x_i, y_j, T)|,
\]

\[
L_2 = \sqrt{\frac{1}{N^2 \sum_{i=1}^{N} \sum_{j=1}^{N} |u(x_i, y_j, T) - u_h(x_i, y_j, T)|^2}}.
\]

### 3.3.1 Transverse magnetic mode

Consider a dielectric cylinder embedded in the free space. By setting the center of the cylinder at \((0, 0)\), we denote the radius to be \( r_0 \). We assign \( \epsilon_1 = \mu_1 = 1 \) to be the relative parameters of vacuum while \( \epsilon_2 \) and \( \mu_2 \) are the relative dielectric parameters of the cylinder. The transverse magnetic (TM) electromagnetic wave is scattered by a time-harmonic incident plane unit wavelength wave of the form \([8, 33]\)

\[
E_z^{\text{inc}} = e^{-i(k_1 x + \omega t)},
\]

where \( k_1 = \omega \sqrt{\mu_1 \epsilon_1} \) is the propagation constant in the free-space medium, and \( \omega \) is the angular frequency. Then the exact solution for such incident waves is computed by using
the summed-series technique \[33, 44\] as the follows

\[
E_z(x, y, t) = E_z(r, \theta, t) = e^{-i\omega t} \left\{ \begin{array}{ll}
\sum_{n=-\infty}^{\infty} A_n J_n (k_2 r) e^{in\theta}, & r \leq r_0, \\
\sum_{n=-\infty}^{\infty} (i^n J_n (k_1 r) + B_n H_n^{(2)} (k_1 r)) e^{in\theta}, & r > r_0,
\end{array} \right.
\]

(3.3.2)

where \((r, \theta)\) is the polar coordinate at \((x, y)\), \(k_2 = \omega \sqrt{\mu_2 \varepsilon_2}\) is the propagation constant for the dielectric cylinder, \(J_n\) and \(H_n^{(2)}\) represent, respectively, the \(n\)th order Bessel function of the first kind and the Hankel function of the second kind, and the wave amplitude coefficients equal to

\[
A_n = i^{-n} (k_1/\mu_1) J_n'(k_1 r_0) H_n^{(2)'}(k_1 r_0) - (k_1/\mu_1) H_n^{(2)'}(k_1 r_0) J_n(k_1 r_0),
\]

(3.3.3)

\[
B_n = i^{-n} (k_1/\mu_1) J_n'(k_1 r_0) J_n(k_2 r_0) - (k_1/\mu_2) J_n'(k_2 r_0) J_n(k_1 r_0).
\]

(3.3.4)

Then the radial component and angular component of the total magnetic field are given as

\[
H_r(r, \theta, t) = e^{-i\omega t} \left\{ \begin{array}{ll}
\frac{-i}{\omega \mu_2 r} \sum_{n=-\infty}^{\infty} \sin n A_n J_n (k_2 r) e^{in\theta}, & r \leq r_0, \\
\frac{-i}{\omega \mu_1 r} \sum_{n=-\infty}^{\infty} \sin (i^n J_n (k_1 r) + B_n H_n^{(2)} (k_1 r)) e^{in\theta}, & r > r_0,
\end{array} \right.
\]

(3.3.5)

\[
H_\theta(r, \theta, t) = e^{-i\omega t} \left\{ \begin{array}{ll}
\frac{ik_2}{\omega \mu_2} \sum_{n=-\infty}^{\infty} A_n J_n'(k_2 r) e^{in\theta}, & r \leq r_0, \\
\frac{ik_1}{\omega \mu_1} \sum_{n=-\infty}^{\infty} \left( i^n J_n'(k_1 r) + B_n H_n^{(2)}'(k_1 r) \right) e^{in\theta}, & r > r_0.
\end{array} \right.
\]

(3.3.6)

By using the coordinate transformation, exact solutions for \(H_x\) and \(H_y\) are determined as the follows

\[
H_x = \cos \theta H_r - \sin \theta H_\theta, \quad H_y = \sin \theta H_r + \cos \theta H_\theta.
\]

(3.3.7)

In the following tests, we assign the radius of the cylinder to be \(r_0 = 0.4\) and angular frequency to be \(\omega = 2\pi\). Two cases will be studied. In the first case, we take \(\varepsilon_2 = 10\) and
\( \mu_2 = 1 \). Since \( \mu_1 = \mu_2 \), we have that all three components \( E_z, H_x, \) and \( H_y \) being continuous. In the second case, we choose \( \epsilon_2 = \mu_2 = 10 \). Then the magnetic components \( H_x \) and \( H_y \) are discontinuous across the interface \( \Gamma \), while \( E_z \) is still continuous. We note that the Bessel functions are singular at the origin \((0,0)\). To avoid possible numerical problems, we need to make sure that the origin is not sampled in our grids for the MIBTD method. To this end, the mesh size \( N \) is chosen as an even integer.

We first study the stability of our proposed method with a large enough stopping time \( T = 10 \). It is well known that the Courant-Friedrichs-Lewy (CFL) stability condition for the FDTD algorithm can be expressed as [26]

\[
\Delta t \leq C_m \frac{h}{v_{\text{max}} \sqrt{d}}, \tag{3.3.8}
\]

where \( d = 2 \) is the dimension number, and the maximum velocity of the propagating wave is defined as \( v_{\text{max}} = \max \left\{ \frac{1}{\sqrt{\mu_1 \epsilon_1}}, \frac{1}{\sqrt{\mu_2 \epsilon_2}} \right\} \). Since we have \( \mu_1 = \epsilon_1 = 1 \) in both cases, the maximum velocity is fixed to be \( v_{\text{max}} = 1 \). The value of the CFL constant \( C_m \) is determined by both the spatial and temporal discretizations. The procedure to numerically identify this CFL constant has been detailed in [8]. Essentially, we need to search for a critical number of time steps, \( N_t \), which just remains stable. The numerically detected CFL value \( C_m \) and critical \( N_t \) of the MIBTD algorithm are reported in Table 3.1. For the smooth problem, i.e., Case 1, \( C_m \) goes to a number around 1.36 as \( h \) approaches zero. The CFL number \( C_m \) takes a smaller number when the solutions are discontinuous in Case 2.

We next investigate the accuracy of MIBTD method with a stopping time \( T = 1 \). To ensure stability, we choose \( C_m = 0.7 \). For each grid, the \( \Delta t \) values can be correspondingly determined. The results of MIBTD method is reported in the Table 3.2. Here only the errors in the \( E_z \) component are listed in both \( L_\infty \) and \( L_2 \) norms. The numerical errors of all three components \( E_z, H_y, \) and \( H_x \) are plotted in Fig. 3.4. Successive mesh refinements are considered, so that we can calculate the numerical orders after each refinement. We can see
Table 3.1: Critical CFL number of the MIBTD algorithm for the TM mode in the dielectric interface problems.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>$N_t$ Critical</th>
<th>$C_m$</th>
<th>$N_t$ Critical</th>
<th>$C_m$</th>
</tr>
</thead>
<tbody>
<tr>
<td>20</td>
<td>1.05E-1</td>
<td>101</td>
<td>1.3302</td>
<td>99</td>
<td>1.3571</td>
</tr>
<tr>
<td>40</td>
<td>5.13E-2</td>
<td>197</td>
<td>1.3999</td>
<td>195</td>
<td>1.4142</td>
</tr>
<tr>
<td>80</td>
<td>2.53E-2</td>
<td>396</td>
<td>1.4106</td>
<td>394</td>
<td>1.4178</td>
</tr>
<tr>
<td>160</td>
<td>1.26E-2</td>
<td>825</td>
<td>1.3628</td>
<td>816</td>
<td>1.3778</td>
</tr>
<tr>
<td>320</td>
<td>6.27E-3</td>
<td>1654</td>
<td>1.3638</td>
<td>1956</td>
<td>1.1532</td>
</tr>
</tbody>
</table>

Table 3.2: Numerical convergence test of the MIBTD algorithm for the dielectric interface problems in the TM mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>Case 1: $(\epsilon_2, \mu_2) = (10, 1)$</th>
<th>Case 2: $(\epsilon_2, \mu_2) = (10, 10)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$L_\infty$ error</td>
<td>Order</td>
</tr>
<tr>
<td>20</td>
<td>1.05E-1</td>
<td>9.63E-1</td>
<td>1.89E-1</td>
</tr>
<tr>
<td>40</td>
<td>5.13E-2</td>
<td>2.67E-1</td>
<td>1.85</td>
</tr>
<tr>
<td>80</td>
<td>2.53E-2</td>
<td>6.71E-2</td>
<td>1.99</td>
</tr>
<tr>
<td>160</td>
<td>1.26E-2</td>
<td>1.67E-2</td>
<td>2.00</td>
</tr>
<tr>
<td>320</td>
<td>6.27E-3</td>
<td>4.20E-3</td>
<td>1.99</td>
</tr>
</tbody>
</table>

that our designed method delivers a second order convergence in these studies, except when grids are too coarse in beginning refinements of the Case 2. This is because the wavenumber $k_2$ is too large with $\epsilon_2 = \mu_2 = 10$. When one refines the mesh, the MIBTD starts to converge uniformly. The contour plots and slice plots of the MIBTD solutions are shown in Fig. 3.5 and Fig. 3.6, respectively for $(\epsilon_2 = 10, \mu_2 = 1)$ and $(\epsilon_2 = 10, \mu_2 = 10)$. These plots clearly reveal that $E_z$ is $C^1$, $H_y$ and $H_x$ are $C^0$ in the first case; $E_z$ belongs to $C^0$, $H_x$ and $H_y$ are discontinuous across the interface in the latter case. In addition, the contour and slice plots indicate a highly oscillatory solution inside the dielectric cylinder, especially when $(\epsilon_2 = 10, \mu_2 = 10)$. Only high order methods, such as the proposed MIBTD algorithm, can capture such high frequency solutions accurately.
3.3.2 Transverse electric mode

We next consider the transverse electric (TE) mode. The same circular interface and dielectric coefficients as in the TM mode are employed for the TE mode. The incident plane wave is assumed for \( H_z \)

\[
H_z^{\text{inc}} = e^{-i(k_1 x + \omega t)}. \tag{3.3.9}
\]

By using the summed-series technique [33, 44] again, the exact solution for \( H_z \) field is given as the follows

\[
H_z(x, y, t) = H_z(r, \theta, t) = e^{-i\omega t} \begin{cases} 
\sum_{n=-\infty}^{\infty} C_n J_n (k_2 r) e^{i n \theta}, & r \leq r_0, \\
\sum_{n=-\infty}^{\infty} \left( i^{-n} J_n (k_1 r) + D_n H_n^{(2)} (k_1 r) \right) e^{i n \theta}, & r > r_0,
\end{cases} \tag{3.3.10}
\]
Figure 3.5: The MIBTD solution with $N = 160$ at $t = 1$ for the dielectric problem in the TM mode with $(\epsilon_{2},\mu_{2}) = (10,1)$. (a) Contour plot of $E_{z}$. (b) $E_{z}(x,0)$. (c) Contour plot of $H_{y}$. (d) $H_{y}(x,0)$. (e) Contour plot of $H_{x}$. (f) $H_{x}(0,y)$.
Figure 3.6: The MIBTD solution with $N = 160$ at $t = 1$ for the dielectric problem in the TM mode with $(\varepsilon_2, \mu_2) = (10, 10)$. (a) Contour plot of $E_z$. (b) $E_z(x, 0)$. (c) Contour plot of $H_y$. (d) $H_y(x, 0.2453)$. (e) Contour plot of $H_x$. (f) $H_x(0, y)$. 
with the wave amplitude coefficients

\[
C_n = i^{-n} \left( \frac{k_1}{\epsilon_1} J'_n(k_1 r_0) H^{(2)}_n(k_1 r_0) - \frac{k_2}{\epsilon_2} J'_n(k_2 r_0) H^{(2)}_n(k_1 r_0) \right), \quad (3.3.11)
\]

\[
D_n = i^{-n} \left( \frac{k_1}{\epsilon_1} J'_n(k_1 r_0) J_n(k_2 r_0) - \frac{k_2}{\epsilon_2} J'_n(k_2 r_0) J_n(k_1 r_0) \right). \quad (3.3.12)
\]

Then the radial component and angular component of the total electric field are given as

\[
E_r(r, \theta, t) = e^{-i\omega t} \begin{cases} 
\frac{i}{\omega \epsilon_2 r} \sum_{n=-\infty}^{\infty} n C_n J_n(k_2 r) e^{in\theta}, & r \leq r_0, \\
\frac{i}{\omega \epsilon_1 r} \sum_{n=-\infty}^{\infty} \left(i^{-n} J_n(k_1 r) + D_n H^{(2)}_n(k_1 r)\right) e^{in\theta}, & r > r_0,
\end{cases} \quad (3.3.13)
\]

\[
E_\theta(r, \theta, t) = e^{-i\omega t} \begin{cases} 
\frac{-ik_2}{\omega \epsilon_2} \sum_{n=-\infty}^{\infty} C_n J'_n(k_2 r) e^{in\theta}, & r \leq r_0, \\
\frac{-ik_1}{\omega \epsilon_1} \sum_{n=-\infty}^{\infty} \left(i^{-n} J'_n(k_1 r) + D_n H^{(2)}_n'(k_1 r)\right) e^{in\theta}, & r > r_0.
\end{cases} \quad (3.3.14)
\]

By using the coordinate transformation, exact solutions for \(E_x\) and \(E_y\) are determined as the follows

\[
E_x = \cos \theta E_r - \sin \theta E_\theta, \quad E_y = \sin \theta E_r + \cos \theta E_\theta. \quad (3.3.15)
\]

The physical parameters of the present TE mode are chosen as in the TM mode, i.e, \(r_0 = 0.4\) and \(\omega = 2\pi\). We also study two cases. For the first case, we also have \(\epsilon_2 = 10\) and \(\mu_2 = 1\). Nevertheless, unlike the TM mode, the present Maxwell interface problem is discontinuous. In particular, both \(E_x\) and \(E_y\) are discontinuous, while \(H_z\) is still continuous. For the second case, we also choose \(\epsilon_2 = \mu_2 = 10\). It is interesting to note that the present TE case is actually identical to the second case of the TM mode, by simply exchanging \((H_z, E_x, E_y)\) with \((E_z, H_x, H_y)\).

We also investigate the stability of the MIBTD method. The critical CFL numbers based on a stopping time \(T = 10\) are reported in Table 3.3. Comparing with the TM results, the CFL numbers become slightly smaller in the Case 1. For the Case 2, the CFL numbers are
Table 3.3: Critical CFL number of the MIBTD algorithm for the dielectric interface problems in the TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>Case 1: $(\epsilon_2, \mu_2) = (10, 1)$</th>
<th>Case 2: $(\epsilon_2, \mu_2) = (10, 10)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Critical $N_t$</td>
<td>$C$</td>
</tr>
<tr>
<td>20</td>
<td>1.05E-1</td>
<td>112</td>
<td>1.1956</td>
</tr>
<tr>
<td>40</td>
<td>5.13E-2</td>
<td>206</td>
<td>1.3387</td>
</tr>
<tr>
<td>80</td>
<td>2.53E-2</td>
<td>418</td>
<td>1.3364</td>
</tr>
<tr>
<td>160</td>
<td>1.26E-2</td>
<td>904</td>
<td>1.2437</td>
</tr>
<tr>
<td>320</td>
<td>6.27E-3</td>
<td>1826</td>
<td>1.2346</td>
</tr>
</tbody>
</table>

Table 3.4: Numerical convergence test of the MIBTD algorithm for the dielectric interface problems in the TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$h$</th>
<th>Case 1: $(\epsilon_2, \mu_2) = (10, 1)$</th>
<th>Case 2: $(\epsilon_2, \mu_2) = (10, 10)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>$L_\infty$ error</td>
<td>Order</td>
</tr>
<tr>
<td>20</td>
<td>1.05E-1</td>
<td>2.73E-0</td>
<td>1.94</td>
</tr>
<tr>
<td>40</td>
<td>5.13E-2</td>
<td>1.07E-0</td>
<td>1.35</td>
</tr>
<tr>
<td>80</td>
<td>2.53E-2</td>
<td>3.14E-1</td>
<td>1.77</td>
</tr>
<tr>
<td>160</td>
<td>1.26E-2</td>
<td>7.84E-2</td>
<td>2.00</td>
</tr>
<tr>
<td>320</td>
<td>6.27E-3</td>
<td>2.05E-2</td>
<td>1.94</td>
</tr>
</tbody>
</table>

actually identical, because the physical problem is essentially the same.

By taking $T = 1$ and $C_m = 0.7$, the $L_2$ and $L_\infty$ errors in the $H_z$ component of the MIBTD method given in Table 3.4. For a visual comparison, we plot all numerical errors of all components consisting of $H_z$, $E_y$, and $E_x$ in Fig. 3.7. In our proposed method, the convergence begins only when a sufficiently fine mesh is used, due to the impact of discontinuous solution and large wavenumber. The second order convergence is achieved on fine meshes. Moreover, the MIBTD results for Case 2 are identical to those of TM mode Case 2, due to the problem equivalence. Therefore, the contour and slice plots of the MIBTD solutions are depicted in Fig. 3.8 only for Case 1. These figures clearly indicate the loss of regularities of wave solutions due to the interaction with the dielectric interface.
Figure 3.7: Numerical convergence tests for the dielectric interface problems in the TE mode. (a) MIBTD scheme, Case 1 \((\epsilon_2, \mu_2) = (10, 1)\); (b) MIBTD scheme, Case 2 \((\epsilon_2, \mu_2) = (10, 10)\);

### 3.4 Conclusion

In this chapter, we proposed a novel FDTD method based on the MIB algorithm to solve the dielectric interface problems with discontinuous electric and/or magnetic parameters. In the previous approaches, the MIB method reported in [26] is only applicable to the straight interfaces. This approach has been extended to the irregular interfaces as introduced in [55], but it is not suitable and directly applied for the electromagnetic interface problems due to the staggered placement of the field components. To overcome this difficulty, a novel MIB treatment for mixed jump conditions is designed in this work. As a result, a second-order accuracy across the interface is successfully restored based on the numerical results. Also, by applying Runge-Kutta time stepping schemes, the MIBTD method is numerically verified to be conditionally stable.
Figure 3.8: The MIBTD solution with $N = 160$ at $t = 1$ for the dielectric problem in the TE mode with $(\epsilon_2, \mu_2) = (10, 1)$. (a) Contour plot of $H_z$. (b) $E_z(x, 0)$. (c) Contour plot of $E_y$. (d) $H_y(x, 0.3544)$. (e) Contour plot of $E_x$. (f) $H_x(-0.0692, y)$. 
Chapter 4

TIME-DOMAIN MATCHED INTERFACE AND BOUNDARY METHODS FOR DEBYE DISPERSIVE INTERFACE PROBLEMS IN TM MODE

4.1 Introduction

As early discussed in Section 2.2.3, dispersive media feature a frequency-dependent of the field components. As a result, the regularities of the wave solutions change in a time manner. In other words, jump conditions of field solutions are a function of time while their counter parts for dielectric interface problems are time-independent (see Section 3.2.3). Therefore, the proposed method in Chapter 3 for nondispersive media is not appropriate for the dispersive interface problems.

In this chapter, we investigate the first-order Debye media with their constitutive relations described in (2.3.1). The first embedded interface method based on FDTD algorithm for the dispersive interface problems is introduced by Zhao [6] in 2011. However this approach is only designed for the TEM system, i.e. 1D Maxwell’s equations. The higher dimensional problems give rise to many difficulties due to the complicated jump conditions and irregular interfaces. We here present a high order methods for TM mode with Debye dispersive interface. This report is based on our published work [7, 8]. By properly constructing the field relations across the interface, our novel method is able to achieve up to the 6 sixth order accuracy for the straight interfaces and uniformly attain second order converge for the irregular ones.

Based on the ADE approach (see Section 2.3), we obtain the Debye-Maxwell system
(2.5.18)–(2.5.21). For convenience, we replicate them in the following

\[
\frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \frac{\partial E_z}{\partial y}, \quad (4.1.1)
\]

\[
\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \quad (4.1.2)
\]

\[
\frac{\partial D_z}{\partial t} = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}, \quad (4.1.3)
\]

\[
D_z + \gamma \frac{\partial D_z}{\partial t} = \epsilon_0 \epsilon_s E_z + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E_z}{\partial t}. \quad (4.1.4)
\]

The complexity of a dispersive problem over a nondispersive one can be appreciated through governing equations. In the dispersive media, the electric flux density \(D_z\) and the electric field \(E_z\) are related by an ODE in (4.1.4) instead of a scalar relationship as in the nondispersive materials. Across a general dispersive interface, four parameters, i.e., \(\epsilon_s, \epsilon_\infty, \gamma\) and \(\mu\), could be discontinuous. Moreover, since equation (4.1.4) involves time \(t\), the resulting jump conditions at dispersive interfaces are also time dependent.

4.2 Matched and interface boundary (MIB) algorithm

As mentioned in the MIB algorithm in Section 3.2 of the dielectric interface problems, a key idea in the matched interface and boundary (MIB) interface treatment is to decompose 2D jump conditions into one-dimensional (1D) ones along each Cartesian direction. Jump conditions for the field components are obtained on the local coordinate system at first. They, then, will be transformed to the regular grid system via operators (3.2.4) and (3.2.5).

4.2.1 Interface jump conditions in a local coordinate

Consider a 2D domain of a rectangle shape \(\Omega = [a, b] \times [c, d]\). An interface \(\Gamma\) separates the domain \(\Omega\) into two parts \(\Omega^+\) and \(\Omega^-\), see Fig. 4.1. In this paper, we will assume the interface \(\Gamma\) being arbitrary curved and \(C^0\) continuous. For two media on both hand sides
of \( \Gamma \), if one of them is a dispersive medium, we will refer to \( \Gamma \) as a dispersive interface. For simplicity, we will assume that the outside medium \( \Omega^+ \) being the air or vacuum in the present study. We note that the proposed formulation and algorithm can be applied to a more general dispersive interface with two dispersive materials.

Similar to the dielectric interface problems in Chapter 3, we define the jump of a function \( u(x, y) \) at \( \Gamma \) to be \( [u] := u^+ - u^- \). The superscript, \( - \) or \( + \), denotes the limiting value of function from one side or from the other side of the interface. For the present Debye-air dispersive interface, we assume the material equation (4.1.4) in the vacuum \( \Omega^+ \) as well with \( \epsilon_s^+ = \epsilon_s^- = 1 \). Then, the static frequency \( \epsilon_s \) and the high frequency limit \( \epsilon_{\infty} \) in (4.1.4) are both discontinuous across the interface \( \Gamma \). Here, \( \gamma^- \) is a free parameter so that we can assume \( \gamma = \gamma^- = \gamma^+ \) being a constant throughout \( \Omega \). Moreover, the magnetic permeability \( \mu \) could be discontinuous across interface \( \Gamma \). In the positive side, i.e., free space, \( \mu^+ \) is assigned to be either 1 or \( \mu_0 \), depending on what type of Maxwell formalism is considered.

According to (2.6.1), field solutions in both media are related analytically via the jump
conditions

\[ \vec{n} \times (E^+ - E^-) = 0, \vec{n} \cdot (D^+ - D^-) = 0, \vec{n} \times (H^+ - H^-) = 0, \vec{n} \cdot (\mu H^+ - \mu^- H^-) = 0, \]

(4.2.1)

where \( \vec{n} \) is the unit vector normal to the interface, pointing from \( \Omega^- \) into \( \Omega^+ \). We will consider jump conditions (4.2.1) in terms of a local Cartesian coordinate \((\vec{n}, \vec{r}, \vec{z})\) as shown in Fig. 3.2. On such a local grid system, equation (4.2.1) gives rise to the following zeroth order jump conditions

\[ [E_z] = 0, \quad [E_\tau] = 0, \quad [D_n] = 0, \quad [H_z] = 0, \quad [H_\tau] = 0, \quad [\mu H_n] = 0. \] (4.2.2)

The first order conditions in terms of the local coordinate for the \( E_z \) component are achieved in the same approach as in Section 3.2.2, one gets

\[ \left[ \frac{1}{\mu} \frac{\partial E_z}{\partial n} \right] = 0, \quad \left[ \frac{\partial E_z}{\partial \tau} \right] = 0. \] (4.2.3)

For the magnetic components, three first order jump conditions can be similarly derived as in the nondispersive case, see Section 3.2.2

\[ \left[ \frac{\partial H_\tau}{\partial \tau} \right] = 0, \quad \left[ \frac{\partial(\mu H_n)}{\partial \tau} \right] = 0, \quad \left[ \frac{\partial(\mu H_\tau)}{\partial \tau} \right] + \left[ \frac{\partial(\mu H_n)}{\partial n} \right] = 0. \] (4.2.4)

One more first order jump condition is required, which, however, is not readily available. We overcome this difficulty by using some interface auxiliary differential equations (IADEs) [6]. In particular, we assume \([\mu D_z] = \psi(t, x, y)\) for some unknown function \(\psi(t, x, y)\). We multiply the first equation of (3.3.1) by \(\mu\) and take jump operations to it to attain the last jump condition

\[ \left[ \frac{\partial \psi(t, y)}{\partial t} \right] = \left[ \frac{\partial(\mu D_z)}{\partial t} \right] = \left[ \frac{\partial(\mu H_y)}{\partial x} \right] - \left[ \frac{\partial(\mu H_x)}{\partial y} \right]. \] (4.2.5)

We note that the nonhomogeneous term in (4.2.5) is time dependent and unknown.
4.2.2 Interface jump conditions in the Cartesian coordinate

Jump conditions for the $E_z$ component for the dispersive interface problems are similarly to the ones for the nondispersive case in Section 3.2.3. Therefore, we can immediately obtain the zeroth and first order jump conditions for $E_z$ as follows

$$E_z^+ - E_z^- = 0,$$

$$A_x^+ \left( \frac{\partial E_z}{\partial x} \right)^+ + A_y^+ \left( \frac{\partial E_z}{\partial y} \right)^+ - A_x^- \left( \frac{\partial E_z}{\partial x} \right)^- = 0,$$

$$B_x^+ \left( \frac{\partial E_z}{\partial x} \right)^+ + B_y^+ \left( \frac{\partial E_z}{\partial y} \right)^+ - B_y^- \left( \frac{\partial E_z}{\partial y} \right)^- = 0,$$

where

$$A_x^+ = \frac{1}{\mu^+} \cos \theta + \frac{1}{\mu^-} \tan \theta \sin \theta, \quad A_y^+ = \left( \frac{1}{\mu^+} - \frac{1}{\mu^-} \right) \sin \theta, \quad A_x^- = \frac{1}{\mu^-} (\cos \theta + \tan \theta \sin \theta),$$

$$B_x^+ = \left( \frac{1}{\mu^+} - \frac{1}{\mu^-} \right) \cos \theta, \quad B_y^+ = \frac{1}{\mu^-} \cos \theta \cot \theta + \frac{1}{\mu^+} \sin \theta, \quad B_y^- = \frac{1}{\mu^-} (\cos \theta \cot \theta + \sin \theta).$$

By employing a similar idea of getting interface conditions for magnetic fields in the dielectric interface problems, we instantaneously arrive at the zeroth jump conditions for these fields in the current problems

$$C_x^+ H_x^+ + C_y^+ H_y^+ - C_x^- H_x^- = 0,$$

$$D_x^+ H_x^+ + D_y^+ H_y^+ - D_x^- H_x^- = 0,$$

where

$$C_x^+ = (\mu^+ - \mu^-) \cos \theta \sin \theta, \quad C_y^+ = \sin^2 \theta \mu^+ + \cos^2 \theta \mu^-, \quad C_x^- = \mu^-,$$

$$D_x^+ = \sin^2 \theta \mu^- + \cos^2 \theta \mu^+, \quad D_y^+ = (\mu^+ - \mu^-) \sin \theta \cos \theta \quad \text{and} \quad D_x^- = \mu^-.$$

To attain the first order jump conditions for $H_x$ and $H_y$, we again employ the coordinate
transformations defined in (3.2.4) and (3.2.5). For three conditions given in (4.2.4) and together with (4.2.5) based on the IADE, we have

\[ 0 = \left[ \frac{\partial (\mu H_n)}{\partial n} \right] + \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right] = \left[ \frac{\partial (\mu H_x)}{\partial x} \right] + \left[ \frac{\partial (\mu H_y)}{\partial y} \right] \]  \hspace{1cm} (4.2.9)

\[ 0 = \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right] = \sin^2 \theta \left[ \frac{\partial (\mu H_x)}{\partial x} \right] - \cos \theta \sin \theta \left[ \frac{\partial (\mu H_x)}{\partial y} \right] - \sin \theta \cos \theta \left[ \frac{\partial (\mu H_y)}{\partial x} \right] + \cos^2 \theta \left[ \frac{\partial (\mu H_y)}{\partial y} \right], \]  \hspace{1cm} (4.2.10)

\[ 0 = \left[ \frac{\partial (\mu H_n)}{\partial \tau} \right] = -\sin \theta \cos \theta \left[ \frac{\partial (\mu H_x)}{\partial x} \right] + \cos^2 \theta \left[ \frac{\partial (\mu H_x)}{\partial y} \right] - \sin^2 \theta \left[ \frac{\partial (\mu H_y)}{\partial x} \right] + \cos \theta \sin \theta \left[ \frac{\partial (\mu H_y)}{\partial y} \right]. \]  \hspace{1cm} (4.2.11)

One can derive the first order jump conditions for \( H_x \) and \( H_y \) by solving the four equations (4.2.5), (4.2.9), (4.2.10) and (4.2.11)

\[ \left[ \frac{\partial (\mu H_y)}{\partial x} \right] = \cos^2 \theta \frac{\partial \psi}{\partial t} - \sin(2\theta) \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right] \]  \hspace{1cm} (4.2.12)

\[ \left[ \frac{\partial (\mu H_x)}{\partial x} \right] = -\frac{\sin(2\theta)}{2} \frac{\partial \psi}{\partial t} - \cos(2\theta) \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right] \]  \hspace{1cm} (4.2.13)

\[ \left[ \frac{\partial (\mu H_y)}{\partial y} \right] = \frac{\sin(2\theta)}{2} \frac{\partial \psi}{\partial t} + \cos(2\theta) \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right] \]  \hspace{1cm} (4.2.14)

\[ \left[ \frac{\partial (\mu H_x)}{\partial y} \right] = -\sin^2 \theta \frac{\partial \psi}{\partial t} - \sin(2\theta) \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right]. \]  \hspace{1cm} (4.2.15)

On the right sides of these conditions, while \( \psi(t, x, y) \) is time dependent and needs to be updated at each time step, the term \( [\partial H_x/\partial \tau] \) can be further expanded by using the fact that \( [\partial H_x/\partial \tau] = 0 \)

\[ \left[ \frac{\partial (\mu H_x)}{\partial \tau} \right] = (\mu^+ - \mu^-) \left( \frac{\partial H_x}{\partial \tau} \right)^+ + \mu^- \left[ \frac{\partial H_x}{\partial \tau} \right] = (\mu^+ - \mu^-) \left( \sin^2 \theta \left( \frac{\partial H_x}{\partial x} \right)^+ - \cos \theta \sin \theta \left( \frac{\partial H_x}{\partial y} \right)^+ - \sin \theta \cos \theta \left( \frac{\partial H_y}{\partial x} \right)^+ + \cos^2 \theta \left( \frac{\partial H_y}{\partial y} \right)^+ \right). \]  \hspace{1cm} (4.2.16)
Since $\mu$ is a piecewise constant across the interface, one can deduce another relation in $H$ field from the divergence free of magnetic flux density

$$\frac{\partial H_x}{\partial x} = -\frac{\partial H_y}{\partial y} \tag{4.2.17}$$

Note that in the present implementation, equation (4.2.17) is only applied to the positive side. From (4.2.12) – (4.2.17), we attain the finally first order jump conditions for $H_x$ and $H_y$

\begin{align*}
C_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + C_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ + C_{yy}^+ \left( \frac{\partial H_y}{\partial y} \right)^+ + C_{yx}^- \left( \frac{\partial H_x}{\partial x} \right)^- = C_{yx}^+ \left( \frac{\partial H_x}{\partial x} \right)^-, \tag{4.2.18}
D_{xx}^+ \left( \frac{\partial H_x}{\partial x} \right)^+ + D_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + D_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ + D_{yy}^- \left( \frac{\partial H_x}{\partial x} \right)^- = D_{xx}^+ \left( \frac{\partial H_x}{\partial x} \right)^-, \tag{4.2.19}
\hat{C}_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + \hat{C}_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ + \hat{C}_{yy}^+ \left( \frac{\partial H_y}{\partial y} \right)^+ + \hat{C}_{yx}^- \left( \frac{\partial H_x}{\partial x} \right)^- = \hat{C}_{yx}^+ \left( \frac{\partial H_x}{\partial x} \right)^-, \tag{4.2.20}
\hat{D}_{xx}^+ \left( \frac{\partial H_x}{\partial x} \right)^+ + \hat{D}_{xy}^+ \left( \frac{\partial H_x}{\partial y} \right)^+ + \hat{D}_{yx}^+ \left( \frac{\partial H_y}{\partial x} \right)^+ + \hat{D}_{yy}^- \left( \frac{\partial H_x}{\partial x} \right)^- = \hat{D}_{xy}^+ \left( \frac{\partial H_y}{\partial y} \right)^-, \tag{4.2.21}
\end{align*}

where

\begin{align*}
C_{xy}^+ = -\frac{\sin^2(2\theta)}{2} (\mu^+ - \mu^-), C_{yx}^+ = \mu^+ - \frac{\sin^2(2\theta)}{2} (\mu^+ - \mu^-), \\
C_{yy}^+ = \frac{\sin(4\theta)}{2} (\mu^+ - \mu^-), C_{yx}^- = -\cos^2 \theta, C_{yy}^- = \mu^-, \\
D_{xx}^+ = \mu^+ - \cos^2(2\theta)(\mu^+ - \mu^-), D_{xy}^+ = -\frac{\sin(4\theta)}{4} (\mu^+ - \mu^-), D_{yx}^+ = D_{xy}^+, \\
D_{\psi} = \frac{\sin(2\theta)}{2}, D_{xx}^- = \mu^-, \\
\hat{C}_{xy}^+ = \frac{\sin(4\theta)}{4} (\mu^+ - \mu^-), \hat{C}_{yx}^+ = \hat{C}_{xy}^+, \hat{C}_{yy}^+ = \mu^+ - \cos^2(2\theta)(\mu^+ - \mu^-), \\
\hat{C}_{\psi} = -\frac{\sin(2\theta)}{2}, \hat{C}_{yy}^- = \mu^-, \\
\hat{D}_{xx}^+ = -(\mu^+ - \mu^-) \frac{\sin(4\theta)}{2}, \hat{D}_{xy}^+ = \mu^+ - \frac{\sin^2(2\theta)}{2} (\mu^+ - \mu^-), \hat{D}_{yx}^+ = -\frac{\sin^2(2\theta)}{2} (\mu^+ - \mu^-), \\
\hat{D}_{\psi} = \sin^2 \theta, \text{ and } \hat{D}_{xy}^- = \mu^-.
\end{align*}
Jump conditions (4.2.18) and (4.2.19) will be used for the MIB modeling of the magnetic fields along the \( x \) direction. Jump conditions (4.2.20) and (4.2.21) will be applied for evaluating fictitious values of the magnetic fields in the \( y \) direction.

On other other hand, when \( \mu \) is a constant, i.e., \( \mu^+ = \mu^- \), jump conditions for electric and magnetic fields can be greatly simplified. In particular, we have the following conditions for \( E_z \)

\[
\begin{align*}
[E_z] &= 0, \\
\left[ \frac{\partial E_z}{\partial x} \right] &= 0, \\
\left[ \frac{\partial E_z}{\partial y} \right] &= 0. 
\end{align*}
\] (4.2.22)

Moreover, jump conditions for \( H_x \) and \( H_y \) are now decoupled

\[
\begin{align*}
[H_y] &= 0, \\
\left[ \frac{\partial H_y}{\partial x} \right] &= \frac{\partial \psi(t, x, y)}{\partial t} \frac{\cos^2 \theta}{\mu}, \\
\left[ \frac{\partial H_y}{\partial x} \right] &= \frac{\partial \psi(t, x, y) \sin^2 \theta}{\partial t} \frac{1}{\mu}, \\
\end{align*}
\] (for \( H_y \), 4.2.23)

\[
\begin{align*}
[H_x] &= 0, \\
\left[ \frac{\partial H_x}{\partial y} \right] &= -\frac{\partial \psi(t, x, y)}{\partial t} \frac{\sin^2 \theta}{\mu}, \\
\left[ \frac{\partial H_x}{\partial y} \right] &= 0, \\
\end{align*}
\] (for \( H_x \)). (4.2.24)

For the straight interface, without loss of generality, we can assume the interface is placed vertically. In such situation, the normal vector is aligned to the \( x \)-line, which gives us \( \theta = 0 \). That yields the simpler jump conditions for the magnetic fields. Specifically, we have

\[
\begin{align*}
[H_y] &= 0, \\
\left[ \frac{\partial H_y}{\partial x} \right] &= \frac{1}{\mu} \left[ \frac{\partial \psi(t, x, y)}{\partial t} \right], \\
\left[ \frac{\partial H_x}{\partial y} \right] &= 0, \\
\end{align*}
\] (for \( H_y \), 4.2.25)

\[
\begin{align*}
[H_x] &= 0, \\
\left[ \frac{\partial H_x}{\partial y} \right] &= 0, \\
\end{align*}
\] (for \( H_x \)). (4.2.26)

We note that the jump conditions (4.2.23) and (4.2.24) are much simpler than their counterparts (4.2.18) - (4.2.21) in two senses. First, in (4.2.23) and (4.2.24), \( x \) and \( y \) directions are uncoupled, while in (4.2.18) - (4.2.21), \( x \) and \( y \) derivatives are coupled. Second, in (4.2.18) - (4.2.21), \( H_x \) and \( H_y \) are mixed in each condition, while conditions for \( H_x \) and \( H_y \) are unmixed in (4.2.23) and (4.2.24). Nevertheless, all these jump conditions are time dependent and share a common difficulty, i.e., there is an unknown nonhomogeneous term \( \frac{\partial \psi}{\partial t} \), which has to be calculated at each time step. In order to deal with the time dependent, coupled and mixed jump conditions, new MIB methods have to be formulated.
4.2.3 Maxwell-Debye system and MIB time domain algorithm

In this subsection, a new Maxwell-Debye system will be constructed to facilitate the implementation of the proposed jump conditions. For the purpose of calculating $\psi(t, x, y)$, we first multiply (4.1.4) with $\mu$ and then conduct jump operations for it. This gives rise to the following IADE

$$\gamma \frac{\partial \psi(t, x, y)}{\partial t} + \psi(t, x, y) = \epsilon_0 \gamma [\mu \epsilon_\infty \dot{E}_z] + \epsilon_0 [\mu \epsilon_s E_z],$$

(4.2.27)

where $\dot{E}_z = \frac{\partial E_z}{\partial t}$. Since both $E_z$ and $\dot{E}_z$ are continuous across $\Gamma$, the jump operations on the right hand side of (4.2.27) can be rewritten as

$$g(t, x, y) := \epsilon_0 \gamma [\mu \epsilon_\infty \dot{E}_z] + \epsilon_0 [\mu \epsilon_s E_z] = \epsilon_0 \gamma (\mu^+ \epsilon_\infty^+ - \mu^- \epsilon_\infty^-) \dot{E}_z^+ + \epsilon_0 (\mu^+ \epsilon_s^+ - \mu^- \epsilon_s^-) E_z^+$$

(4.2.28)

Note that $g(t, x, y)$ in (4.2.28) can be evaluated from the negative side in $\Omega^-$ as well, i.e., based on $\dot{E}_z^-$ and $E_z^-$. The positive side is used in the present study, because the incident wave propagates from the positive domain $\Omega^+$. With $g(t, x, y)$, (4.2.27) reduces to

$$\gamma \frac{\partial \psi(t, x, y)}{\partial t} + \psi(t, x, y) = g(t, x, y)$$

(4.2.29)

which can be regarded as an ordinary differential equation with respect to time $t$, for given $x$ and $y$ grid locations.

In order to calculate the $g(t, x, y)$ term in the IADE (4.2.29), we propose to utilize $\dot{E}_z$ instead of $D_z$ to formulate a modified Maxwell system for TM modes

$$\frac{\partial E_z}{\partial t} = \dot{E}_z, \quad \frac{\partial H_y}{\partial t} = \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \quad \frac{\partial H_x}{\partial t} = -\frac{1}{\mu} \frac{\partial E_z}{\partial y},$$

$$\epsilon_0 \epsilon_\infty \gamma \frac{\partial \dot{E}_z}{\partial t} = -\epsilon_0 \epsilon_s \dot{E}_z + \gamma \left( \frac{\partial}{\partial x} \left( \frac{1}{\mu} \frac{\partial E_z}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{\mu} \frac{\partial E_z}{\partial y} \right) \right) + \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right).$$

(4.2.30)

It is noted that in (4.2.30), we need to carry out the MIB interface treatment for $E_z$ along...
Figure 4.2: The staggered grid system for dispersive interface problems in TM modes.

both $x$ and $y$ directions. For two magnetic components, only one derivative is involved for each component, i.e., $\frac{\partial H_y}{\partial x}$ and $\frac{\partial H_x}{\partial y}$. Thus, if $\mu$ is a constant, we will enforce $x$ direction jump condition (4.2.23) and $y$ direction jump condition (4.2.24), respectively, for $H_y$ and $H_x$. When $\mu$ is a piecewise constant, a group of jump conditions including Eqs. (4.2.7), (4.2.8), (4.2.18) and (4.2.19) will be applied for $H_y$. And we impose a group of jump conditions including Eqs. (4.2.7), (4.2.8), (4.2.20) and (4.2.21) for $H_x$.

In our computations, a uniform staggered grid system shown in Fig. 4.2 is employed. As an extension of the standard Yee cell, the field components $E_z$ and $\dot{E}_z$ will be computed on the same collocation node, while $H_x$ and $H_y$ will be calculated on staggered positions. Without the loss of generality, we assume that the interface $\Gamma$ will not pass any grid point in the present work. Away from the interface $\Gamma$, the standard central finite differences are employed to discretize spatial derivatives in (4.2.30), while the finite difference weights in the vicinity of the interface shall be modified based on the MIB scheme, whose details will be offered in Section 4.2.4. The classical fourth order Runge-Kutta method (see Section 2.4.3) is employed to integrate both Maxwell-Debye system (4.2.30) and the IADE (4.2.29) with a fixed time increment $\Delta t$, whereas other standard explicit or implicit time stepping methods may also be used for the time integration.

The proposed MIB time-domain (MIBTD) algorithm consists of three major stages in
each fractional step of the Runge-Kutta time stepping. For simplicity, we will illustrate such a general procedure based on the explicit Euler scheme over the time interval \([t_k, t_{k+1}]\). This is because each fractional step of the four stage Runge-Kutta time integration can be regarded as an Euler integration [40]. In the following, we only consider the case with a constant magnetic permeability \(\mu\) in the present algorithm. The case with a piecewise constant \(\mu\) can be similarly treated. First, the jump conditions (4.2.22) will be imposed along both \(x\) and \(y\) directions for \(E_z\). For \(H_y\), the jump conditions (4.2.23) will be enforced along \(x\) direction based on known values of \(\frac{\partial \psi}{\partial t}(t_k, x_o, y_o)\) on some interface point \((x_o, y_o)\). Similarly, the MIB interface treatment will be conducted for \(H_x\) along \(y\) direction based on \(\frac{\partial \psi}{\partial t}(t_k, x_o, y_o)\) values. With these interface treatments, all spatial derivatives involved in (4.2.30) can then be approximated by finite differences with a second order of accuracy. Second, four equations of (4.2.30) are time integrated to generate function values at \(t_{k+1}\). Similarly, based on known \(g(t_k, x_o, y_o)\) values, one integrates the IADE (4.2.29) for \(\psi(t_{k+1}, x_o, y_o)\). Third, to facilitate computations of next step, one needs to calculate \(\frac{\partial \psi}{\partial t}(t_{k+1}, x_o, y_o)\). Since now \(\psi(t_{k+1}, x_o, y_o)\) is known, by using (4.2.29), we actually need to find \(g(t_{k+1}, x_o, y_o) = \epsilon_0 \gamma (\mu^+ \epsilon_\infty^+ - \mu^- \epsilon_\infty^-) \hat{E}_z^+(t_{k+1}, x_o, y_o) + \epsilon_0 (\mu^+ \epsilon_s^+ - \mu^- \epsilon_s^-) E_z^+(t_{k+1}, x_o, y_o)\). Since \((x_o, y_o)\) is off-grid, \(E_z^+(t_{k+1}, x_o, y_o)\) and \(\hat{E}_z^+(t_{k+1}, x_o, y_o)\) are approximated via one-sided extrapolations based on several nearby function values of \(E_z(t_{k+1}, x_i, y_j)\) and \(\hat{E}_z(t_{k+1}, x_i, y_j)\) in the positive domain \(\Omega^+\). Here \((x_i, y_j)\) are some nearby grid nodes. A flowchart summarizing these three stages of the MIB algorithm is shown in Fig. 4.3.

The proposed MIBTD method can be flexibly converted to the dielectric interface problems with \(\epsilon\) being discontinuous across the interface \(\Gamma\). In this case, the governing equations of TM modes (4.2.30) now degenerate to

\[
\begin{align*}
\frac{\partial E_z}{\partial t} &= \hat{E}_z, \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu} \frac{\partial E_z}{\partial x}, \\
\frac{\partial H_x}{\partial t} &= -\frac{1}{\mu} \frac{\partial E_z}{\partial y}, \\
\frac{\partial \hat{E}_z}{\partial t} &= \frac{1}{\epsilon} \left( \frac{\partial}{\partial x} \left( \frac{1}{\mu} \frac{\partial E_z}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{\mu} \frac{\partial E_z}{\partial y} \right) \right),
\end{align*}
\] (4.2.31)
Given $E_z$, $\dot{E}_z$, $H_x$, $H_y$, $g$, and $\frac{\partial \psi}{\partial t}$ values at $t_k$;
Enforce (4.2.22) to determine fictitious values of $E_z$ at $t_k$;
Enforce (4.2.23) to determine fictitious values of $H_y$ at $t_k$;
Enforce (4.2.24) to determine fictitious values of $H_x$ at $t_k$.

Integrate (4.2.30) by the Euler scheme to attain $E_z$, $\dot{E}_z$, $H_x$, $H_y$ values at $t_{k+1}$;
Integrate (4.2.29) by the Euler scheme to attain $\psi$ values at $t_{k+1}$.

Calculate $g$ values at $t_{k+1}$ by using (4.2.28), based on $E_z$ and $\dot{E}_z$ values at $t_{k+1}$;
Calculate $\frac{\partial \psi}{\partial t}$ values at $t_{k+1}$ by using (4.2.29), based on $g$ values at $t_{k+1}$.

**Figure 4.3:** A flowchart of the MIB algorithm based on the explicit Euler scheme over the time interval $[t_k, t_{k+1}]$ for the case of constant magnetic permeability $\mu$.

where no spatial derivatives are involved for $H_x$ and $H_y$. Thus, one only needs to carry out MIB interface treatment for $E_z$ along both Cartesian directions based on the jump conditions (4.2.6) or (4.2.22), depending on the continuous condition of $\mu$. The classical fourth order Runge-Kutta method is also employed to update Maxwell’s equations (4.2.31). This nondispersive MIBTD algorithm preserves essential features of the dispersive MIBTD algorithm.

It is noticed that the hybrid Maxwell system (4.2.31) is different from the standard one discussed in Chapter 3. Based on the numerical verification, the system degenerated from the dispersive interface problem (4.2.31) is only well-suited for the nondispersive interface with constant magnetic parameter $\mu$. If one wants to deal with the discontinuous $\mu$, the approach presented in Chapter 3 is better to be taken into a consideration.
4.2.4 MIB treatment for unmixed jump conditions

When $\mu$ is piecewise constant, the jump conditions of electric and magnetic fields are now the mixed ones. Therefore, the fictitious value determination of $H_x$ and $H_y$ has to be conducted simultaneously. The MIB treatment for the mixed jump conditions case has been already offered in Section 3.2.4.

We here only consider the MIB treatments for the case with $\mu$ being a constant. In this instance, the jump conditions for electric and magnetic fields are unmixed ones, i.e., only one field component is involved in jump condition (4.2.22), (4.2.23) or (4.2.24). Moreover, these conditions are all one-dimensional ones. For simplicity, we demonstrate only the MIB enforcement of (4.2.22) for $E_z$ here. The jump conditions (4.2.23) and (4.2.24) for $H_y$ and $H_x$ can be similarly treated. We classify a Lipschitz continuous interface as a smooth one or a sharp one. Different MIB treatments are required to handle those interfaces.

4.2.4.1 Smooth interface

Here, a smooth interface is referred to a $C^1$ continuous curve with no sharp edge. The regular MIB method [26, 34] will be used in this situation. The standard high order central finite difference approximation will be carried out away from the interface. The finite difference weights of nodes in the vicinity of the interface, i.e., the so-called irregular points, shall be modified in order to satisfy jump conditions. A universal rule here is that to approximate function or its derivatives on one side of interface, one never directly refers to function values from the other side. Instead, in the MIB scheme, fictitious values from the other side of the interface will be used.

For example, suppose that $(x_i, y_j)$ belongs to $\Omega^+$ and $(x_{i+1}, y_j)$ belongs to $\Omega^-$. See Fig. 4.4. Denote the function value and fictitious value of $E_z$ at the node $(x_i, y_j)$ as $E_{i,j}$ and $f_{i,j}$, respectively. The second order finite difference approximation to the double $x$ derivative
Figure 4.4: Illustration of the MIB grid partition for a smooth interface. Filled circles: grid nodes; Open circles: fictitious nodes; Triangle: interface node.

The term in \((4.2.30)\) will be modified to be

\[
\left. \frac{\partial^2 E_z}{\partial x^2} \right|_{x_i,y_j} \approx \frac{E_{i-1,j} - 2E_{i,j} + f_{i+1,j}}{\Delta x^2}, \quad \left. \frac{\partial^2 E_z}{\partial x^2} \right|_{x_{i+1},y_j} \approx \frac{f_{i,j} - 2E_{i+1,j} + E_{i+2,j}}{\Delta x^2}. \tag{4.2.32}
\]

In these discretizations, the central difference approximation at a given node involves two neighboring nodes. For a smooth interface with a small curvature, one can usually guarantee that one of the two neighboring nodes is from the same sub-domain as the center node. As a result, the standard MIB scheme is always applicable in this situation.

We determine two fictitious values, \(f_i\) and \(f_{i+1}\), by discretizing two jump conditions (4.2.22) in the same manner of Eq. (4.2.32), i.e., never referring to function values across the interface

\[
w_{0,1}^+ E_{i-1,j} + w_{0,2}^+ E_{i,j} + w_{0,3}^+ f_{i+1,j} = w_{0,1}^- f_{i,j} + w_{0,2}^- E_{i+1,j} + w_{0,3}^- E_{i+2,j} + [E]_{o,j}, \tag{4.2.33}
\]

\[
w_{1,1}^+ E_{i-1,j} + w_{1,2}^+ E_{i,j} + w_{1,3}^+ f_{i+1,j} = w_{1,1}^- f_{i,j} + w_{1,2}^- E_{i+1,j} + w_{1,3}^- E_{i+2,j} + \left[ \frac{\partial E}{\partial x} \right]_{o,j}. \tag{4.2.34}
\]

where \(w_{i,k}^-\) and \(w_{i,k}^+\) for \(k = 1,2 \text{ and } 3\) and \(l = 0,1\) are one-sided finite difference weights, respectively, for left and right subdomains. Here the subscript \(l\) represents the interpolation
(l = 0) and the first order derivative approximation (l = 1), and k is for grid index. One-sided approximations involving 2 grid nodes in one side are used to ensure a sufficiently high accuracy. Here \([E]_{o,j}\) and \([\partial E/\partial x]_{o,j}\) are denoted as the zeroth and first order jump of \(E_z\) at interface node \((x_o, y_j)\). Both jump values are vanishing in the present work. However, we choose to present the MIB scheme in such a general way so that it can be readily applied to more complicated occasion.

Algebraically, Eqs. (4.2.33) and (4.2.34) can be translated equivalently into the following matrix system form

\[
W \cdot F = C \cdot U, \quad (4.2.35)
\]

where

\[
W = \begin{bmatrix}
-w_{0,1}^{-} & w_{0,3}^{+} \\
-w_{1,1}^{-} & w_{1,3}^{+}
\end{bmatrix},
F = \begin{bmatrix}
f_{i,j} \\
f_{i+1,j}
\end{bmatrix},
C = \begin{bmatrix}
-w_{0,1}^{+} & -w_{0,2}^{+} & w_{0,2}^{-} & w_{0,3}^{-} & 1 & 0 \\
-w_{1,1}^{+} & -w_{1,2}^{+} & w_{1,2}^{-} & w_{1,3}^{-} & 0 & 1
\end{bmatrix},
\]

and

\[
U = \begin{bmatrix}
E_{i-1,j}, E_{i,j}, E_{i+1,j}, E_{i+2,j}, [E]_{o,j}, \left[\frac{\partial E}{\partial x}\right]_{o,j}\end{bmatrix}^T. \quad (4.2.36)
\]

Then the fictitious values \(F = [f_{i,j}, f_{i+1,j}]^T\) can be determined as follows

\[
F = W^{-1} \cdot C \cdot U. \quad (4.2.37)
\]

Formulation in (4.2.37) means that \(f_{i,j}\) and \(f_{i+1,j}\) are actually linear combinations in terms of the corresponding values \(E_{i-1,j}, E_{i,j}, E_{i+1,j}, E_{i+2,j}, [E]_{o,j}\) and \([\partial E/\partial x]_{o,j}\). The solved coefficients \(W^{-1} \cdot C\) will be referred as representation coefficients. By substituting \(f_{i,j}\) and \(f_{i+1,j}\) into Eq. (4.2.32), a second order finite difference discretization of the \(x\) derivative is constructed. The MIB treatment along the \(y\) direction can be similarly conducted. Finally, we note that the MIB interface matching needs only be carried out once at the beginning. The representation coefficients can then be used in all subsequent time steps [26].

In general, higher order finite difference approximation requires more fictitious points.
For instance, the general \((2M)\)th order central finite difference approximations require a total of \(2M\) fictitious points on both sides of the interface. To determine these fictitious values, function values of a total of \(2L\) grid points will be involved in the discretizations of the jump conditions. At the first step, we determine two fictitious values \(f_i\) and \(f_{i+1}\) in the same manner as of Eqs. (4.2.33) and (4.2.34) to get

\[
\sum_{k=1}^{L} w_{0,k}^{-} E_{i-L+k} + w_{0,L+1}^{-} f_{i+1} + [E]_{o,j} = w_{0,1}^{+} f_i + \sum_{k=2}^{L+1} w_{0,k}^{+} E_{i+k-1}, \tag{4.2.38}
\]

\[
\sum_{k=1}^{L} w_{1,k}^{-} E_{i-L+k} + w_{1,L+1}^{-} f_{i+1} + \left[ \frac{\partial E}{\partial x} \right]_{o,j} = w_{1,1}^{+} f_i + \sum_{k=2}^{L+1} w_{1,k}^{+} E_{i+k-1}, \tag{4.2.39}
\]

To achieve the fourth order accuracy, we determine two more fictitious values by enforcing two jump conditions (4.2.22) again,

\[
\sum_{k=1}^{L} \tilde{w}_{0,k}^{-} E_{i-L+k} + \tilde{w}_{0,L+1}^{-} f_{i+1} + \tilde{w}_{0,L+2}^{-} f_{i+2} + [E]_{o,j} = \tilde{w}_{0,1}^{+} f_{i-1} + \tilde{w}_{0,2}^{+} f_i + \sum_{k=3}^{L+2} \tilde{w}_{0,k}^{+} E_{i+k-2},
\]

\[
\sum_{k=1}^{L} \tilde{w}_{1,k}^{-} E_{i-L+k} + \tilde{w}_{1,L+1}^{-} f_{i+1} + \tilde{w}_{1,L+2}^{-} f_{i+2} + \left[ \frac{\partial E}{\partial x} \right]_{o,j} = \tilde{w}_{1,1}^{+} f_{i-1} + \tilde{w}_{1,2}^{+} f_i + \sum_{k=3}^{L+2} \tilde{w}_{1,k}^{+} E_{i+k-2},
\]

where the finite difference weights \(\tilde{w}_{j,k}^{-}\) and \(\tilde{w}_{j,k}^{+}\) are different from those in Eqs. (4.2.38) and (4.2.39) because they involve a different set of grid points which includes two more fictitious points at \(x_{i-1}\) and \(x_{i+2}\). From these two equations, two new unknowns \(f_{i-1}\) and \(f_{i+2}\) can be determined, since \(f_i\) and \(f_{i+1}\) are known. With these four fictitious values, standard fourth order central finite difference approximations can be evaluated at either \(y_i\) or \(y_{i+1}\), in a manner similar to Eq. (4.2.32). This gives rise to a fourth order MIB method.

By iteratively determining two more fictitious points at each step, finally we can attain \(2M\) fictitious points for a \((2M)\)th order central finite difference approximation across the interface. For the present straight interface problem, such a procedure can be carried out systematically, and is thus of arbitrarily high order in principle. Numerically, the order of
The accuracy of the MIB method is determined by $2M$ at regular grid points, while it is limited by the parameter $L$ at irregular points.

### 4.2.4.2 Sharp interface

Due to the presence of a sharp corner, we may not be able to guarantee that at least one of the two neighboring nodes involved in the central difference approximation is located in the same sub-domain of the center node. See Fig. 4.5. The same situation may still hold, even if the mesh is refined in both the $x$ and $y$ directions. Note that such a difficulty cannot be handled by the original MIB method [26, 34], because it violates the universal rule of this method that the function value and its derivatives should be approximated on one side of the interface. Fortunately, this obstacle can be resolved by the double layer MIB scheme developed in [57].

To illustrate the idea, we suppose that a grid node $(x_i, y_j)$ belongs to the sub-domain $\Omega^+$ while grid nodes $(x_{i-1,j}, y_j)$ and $(x_{i+1,j}, y_j)$ belong to the sub-domain $\Omega^-$. See Fig. 4.5. Consequently, both neighboring nodes of $(x_i, y_j)$ along $x$-direction belong to a different sub-domain.

Therefore, the discretization of $E_z$ at $(x_i, y_j)$ involves only one main grid node and two
fictitious nodes, whereas the discretizations of this field at \((x_{i-1}, y_j)\) or \((x_{i+1}, y_j)\) are still the same as in (4.2.32)

\[
\frac{\partial^2 E_z}{\partial x^2}\bigg|_{x_{i-1},y_j} \approx \frac{E_{i-2,j} - 2E_{i-1,j} + \tilde{f}_{i,j}}{\Delta x^2}, \quad \frac{\partial^2 E_z}{\partial x^2}\bigg|_{x_{i},y_j} \approx \frac{f_{i-1,j} - 2E_{i,j} + f_{i+1,j}}{\Delta x^2}
\]

\[
\frac{\partial^2 E_z}{\partial x^2}\bigg|_{x_{i+1},y_j} \approx \frac{\hat{f}_{i,j} - 2E_{i+1,j} + E_{i+1,j}}{\Delta x^2}
\]

Note that, \(\tilde{f}_{i,j}\) and \(\hat{f}_{i,j}\) are two fictitious points located at the same grid node \((x_i, y_j)\) and they could take different values. Similar to the original MIB method, fictitious values are determined by discretizing two jump conditions (4.2.22). In the traditional MIB, these jump conditions are imposed only at one interface location for solving two fictitious values. But the double layer MIB method [57] will enforce the jump conditions at two consecutive interface locations for the purpose of evaluating four fictitious values at the same time. Referring to Fig. 4.5, two jump conditions (4.2.22) are discretized at two adjacent interface positions \((x_{o1}, y_j)\) and \((x_{o2}, y_j)\)

\[
\begin{align*}
\tilde{w}_{0,1}^{-} E_{i-2,j} + \tilde{w}_{0,2}^{-} E_{i-1,j} + \tilde{w}_{0,3}^{-} \tilde{f}_{i,j} &= w_{0,1}^{+} f_{i-1,j} + w_{0,2}^{+} E_{i,j} + w_{0,3}^{+} f_{i+1,j} - [E]_{o1,j} \quad (4.2.41) \\
\tilde{w}_{1,1}^{-} E_{i-2,j} + \tilde{w}_{1,2}^{-} E_{i-1,j} + \tilde{w}_{1,3}^{-} \tilde{f}_{i,j} &= w_{1,1}^{+} f_{i-1,j} + w_{1,2}^{+} E_{i,j} + w_{1,3}^{+} f_{i+1,j} - \left[ \frac{\partial E}{\partial x} \right]_{o1,j} \quad (4.2.42) \\
\tilde{w}_{0,1}^{+} f_{i-1,j} + \tilde{w}_{0,2}^{+} E_{i,j} + \tilde{w}_{0,3}^{+} f_{i+1,j} &= \tilde{w}_{0,1}^{-} \hat{f}_{i,j} + \tilde{w}_{0,2}^{-} E_{i+1,j} + \tilde{w}_{0,3}^{-} E_{i+2,j} + [E]_{o2,j} \quad (4.2.43) \\
\tilde{w}_{1,1}^{+} f_{i-1,j} + \tilde{w}_{1,2}^{+} E_{i,j} + \tilde{w}_{1,3}^{+} f_{i+1,j} &= \tilde{w}_{1,1}^{-} \hat{f}_{i,j} + \tilde{w}_{1,2}^{-} E_{i+1,j} + \tilde{w}_{1,3}^{-} E_{i+2,j} + \left[ \frac{\partial E}{\partial x} \right]_{o2,j} \quad (4.2.44)
\end{align*}
\]

where the finite difference weights \(\tilde{w}_{l,k}^{-}, w_{l,k}^{+}, \tilde{w}_{l,k}^{+}\) and \(\hat{w}_{l,k}^{-}\) for \(k = 1, 2\) and \(3\) and \(l = 0, 1\) are defined similarly as in the smooth interface case. Here \([E]_{o1,j}, [\frac{\partial E}{\partial x}]_{o1,j}, [E]_{o2,j}\) and \([\frac{\partial E}{\partial x}]_{o2,j}\) are denoted as the zeroth and first order jumps of \(E_z\) at interface nodes \((x_{o1}, y_j)\) and \((x_{o2}, y_j)\).

We again use the matrix language to translate Eqs. (4.2.41), (4.2.42), (4.2.43) and (4.2.44) into the following form

\[
W \cdot F = C \cdot U, \quad (4.2.45)
\]
where

\[
W = \begin{bmatrix}
-w_{0,1}^+ & \tilde{w}_{0,3}^- & 0 & -w_{0,3}^+ \\
-w_{1,1}^+ & \tilde{w}_{1,3}^- & 0 & -w_{1,3}^+ \\
\tilde{w}_{0,1}^- & 0 & -\tilde{w}_{0,1}^- & \tilde{w}_{0,3}^+ \\
\tilde{w}_{1,1}^- & 0 & -\tilde{w}_{1,1}^- & \tilde{w}_{1,3}^+
\end{bmatrix},
F = \begin{bmatrix}
f_{i-1,j} \\
f_{i,j} \\
f_{i+1,j}
\end{bmatrix},
\]

\[
C = \begin{bmatrix}
-\tilde{w}_{0,1}^- & -\tilde{w}_{0,2}^- & \tilde{w}_{0,2}^+ & 0 & 0 & -1 & 0 & 0 & 0 \\
-\tilde{w}_{1,1}^- & -\tilde{w}_{1,2}^- & \tilde{w}_{1,2}^+ & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & -\tilde{w}_{0,2}^- & \tilde{w}_{0,2}^+ & \tilde{w}_{0,3}^- & 0 & 0 & 1 & 0 \\
0 & 0 & -\tilde{w}_{1,2}^- & \tilde{w}_{1,2}^+ & \tilde{w}_{1,3}^- & 0 & 0 & 0 & 1
\end{bmatrix},
\]

and

\[
U = \begin{bmatrix}
E_{i-2,j}, E_{i-1,j}, E_{i,j}, E_{i+1,j}, E_{i+2,j}, [E]_{o1,j}, \left[ \frac{\partial E}{\partial x} \right]_{o1,j}, [E]_{o2,j}, \left[ \frac{\partial E}{\partial x} \right]_{o2,j}\end{bmatrix}^T.
\]

Then fictitious values can be easily found as follows

\[
F = W^{-1} \cdot C \cdot U.
\]

Equation (4.2.47) implies that the fictitious values are the linear combinations of the function values and physical jumps. With these expansions of the fictitious values, one can discretize the second derivative of \(E_z\) in (4.2.40) with a second order of accuracy. The MIB treatment for the \(y\) grid line can be similarly carried out.

### 4.3 Numerical Experiments

In this section, we investigate the performance of the proposed MIBTD method for both straight and curved interfaces. In all studies, the initial waves are defined at an initial time \(t = 0\). The computational process is conducted in \(N_t\) steps, until a stopping time \(T\); which yield a time increment \(\Delta t = T/N_t\). Numerical error \(L_\infty\) norm will be reported in all examples.
4.3.1 Straight interfaces

In all examples for this case, a straight air-water interface is assumed at \( x = \xi \) within a rectangular domain \([a, b] \times [c, d]\). Since the media are homogeneous along \( y \) direction, the discretization parameters in the \( y \) direction, i.e., the number of grid nodes \( N_y \) and the half stencil width \( M_y \), will be chosen to be large enough and will be fixed in each example. Whereas, different \( N_x \) and \( M_x \) will be explored to numerically test the order of convergence for the proposed algorithm. Sufficiently small time increments \( \Delta t \) will be employed in all cases so that the approximation error is mainly due to the spatial discretization.

4.3.1.1 Example 1: Planar incident wave

In our first example, the domain dimensions are chosen as \( a = c = 0 \) mm and \( b = d = 30 \) mm, with the interface location \( \xi = 7.5\pi \) mm. A dispersive water medium is assumed in the right subdomain with \( \epsilon_s = 81, \epsilon_\infty = 1.8 \), and \( \tau = 9.4 \) ps [6, 19]. An incident pulse of the form \( E_z(x, y, t) = \exp\left(-\left(x + 15 - c_0 t\right)^2/(2\alpha^2)\right) \) is imposed as the boundary condition at the left boundary \( x = a \). Here \( \alpha = 2.5 \) mm and \( c_0 \) is the speed of light in air. Since the incident wave is normal with respect to the interface, the electromagnetic wave solutions are actually invariant along \( y \) direction, see Fig. 4.7. For simplicity, periodic conditions will be assumed on the top boundary \( y = d \) and bottom boundary \( y = c \). The computation will stop before the transmitted wave hits the right boundary \( x = b \). In this way, the electromagnetic fields remain to be negligible at \( x = b \). Consequently, this boundary can be assumed to be perfectly electric conducting (PEC) for simplicity (see Section 2.6). In the following tests, the \( y \) direction discretization parameters are fixed to be \( N_y = 10 \) and \( M_y = 4 \).

We first study the reflection coefficient of the air-water interface by considering the second order MIBTD or MIBTD2, in which we set \( M_x = 1 \) and \( L = 2 \). The number of \( x \) grid nodes for \( E_z \) is chosen as \( N_x = 801 \) and the time increment is set to be \( \Delta t = 0.025 \) ps for a total of 10000 steps. The time histories of \( E_z \) are tracked at two locations along one horizontal
Figure 4.6: The reflection coefficient at an air-water interface for the straight interface case in the Debye dispersive interface problems.

line $y = \text{const}$. One location is near the left boundary $x = a$, while another is to the left of the interface $x = \xi$. Through a proper truncation, this yields two time domain samplings for incident and reflected pulses, respectively. The reflection coefficient can then be calculated as the ratio of the Fourier transform of the reflected wave over that of the incident wave. The reflection coefficient of the MIBTD2 is plotted against the analytical one [19] in Fig. 4.6. Obviously, our numerical results agree with the analytical one over a wide range of frequencies.

To rigorously examine the proposed higher order MIBTD methods, we next conduct a numerical convergence analysis. The parameters for the higher order MIBTD are chosen as: $(M_x, L) = (2, 4)$ and $(3, 6)$, respectively, for the MIBTD4 and MIBTD6. The implementation of the PEC boundary condition in the high order finite difference methods has been discussed in [45]. In the present work, a stop time $t = 140\ \text{ps}$ is chosen, which is short enough such that both reflected and transmitted pulses have not reached the horizontal boundaries, see Fig. 4.7. We note again that our incident wave here is constant with respect to the $y$ direction. The same conclusion holds for $E_z, H_y$ and $H_x$. In fact, all values of $H_x$ are equal to zero throughout our computations, because the change of $H_x$ is determined by the $y$
Figure 4.7: The MIBTD6 solution with $N_x = 201$ and $N_y = 10$ at $t = 140$ ps for the Example 1 of the straight interface case in the Debye dispersive interface problems. Left: $E_z$; Right: $H_y$.

partial derivative of $E_z$ in (4.1.1). Thus, only non-trivial $E_z$ and $H_y$ solutions are plotted in Fig. 4.7.

In the present example, a reference solution is generated by employing the MIBTD6 with a very dense grid $N_x = 12801$ and a small enough $\Delta t$. Convergence analysis can then be conducted by considering mesh refinements based on nodes that are also sampled in the reference solution. Specifically, the minimal requirement for a tested mesh size $N_x$ is that $N_x - 1$ is an integer factor of 12800. For example, when $N_x = 1601$, the reference solution needs to be downsampled with a rate 8 along $x$ direction, i.e., keeping one $E_z$ value in every eight $E_z$ values. The downsampled reference solution can then be compared with the numerical solution to compute the maximal error for $E_z$. We note that since the $H_y$ nodes are staggered to the $E_z$ nodes, the present convergence analysis is not applicable to $H_y$.

The maximal errors in $E_z$ of the MIBTD methods are depicted Fig. 4.8. The results of the classical dispersive FDTD, obtained via the Yee scheme discussed in Section 2.5, are also included for a comparison. In all cases, the numerical errors based on different mesh size $N = N_x$ are plotted as dashed lines. A linear least-squares fitting [34] is then conducted in the log-log scale. The fitted convergence lines are shown as solid lines in Fig. 4.8. Moreover, the fitted slope essentially represents the numerical convergence rate $r$ of the
scheme. The traditional dispersive algorithms fail to deliver high accuracy because of the loss of regularities in wave solutions near the interface. In particular, it can be seen from Fig. 4.7 that $E_z$ is $C^1$ continuous across the interface, but $H_y$ is only $C^0$ continuous. Moreover, the interface location $\xi$ is generally not located on grid during the mesh refinements, because it is an irrational number. Therefore, the conventional FDTD algorithm degrades to the first order of accuracy, i.e., $r = 1.18$ in Fig. 4.8. Nevertheless, after the implementing the MIB interface treatments, higher order convergence can be restored. In the present study, the numerical order $r$ of the MIBTD2, MIBTD4, and MIBTD6 methods is found to be 2.12, 4.32, and 5.74, respectively, which confirms the theoretical orders of two, four, and six.

4.3.1.2 Example 2: Gaussian-Gaussian initial wave

Since all solutions in the Example 1 are invariant along the $y$ direction, the two-dimensional (2D) result of the Example 1 is very close to its counterpart in one-dimension (1D), reported in our previous study [6]. We thus consider a real 2D study in the present example. The domain is chosen as $a = 0$ mm, $b = 12$ mm, $c = 0$ mm, and $d = 10$ mm. The interface is located at $\xi = 3\pi$ mm and the same Debye parameters as in Example 1 are used for the
Figure 4.9: The MIBTD4 solution for the Example 2 of the straight interface case in the Debye dispersive interface problems with $N_x = 201$ and $N_y = 51$ at $t = 60$ ps. Top left: $E_z$; Top right: $H_y$; Bottom: $H_x$.

dispersive material. We introduce a Gaussian-Gaussian initial wave solution at time $t = 0$ for $E_z$, while the initial solutions for $H_x$ and $H_y$ are assumed to be zero. In particular, we set $E_z(x, y, 0) = \exp\left(-\left((x-x_c)^2 + (y-y_c)^2\right)/(2\alpha^2)\right)$ with $x_c = y_c = (d-c)/2$. The Gaussian window parameter is set as $\alpha = 0.5$ mm, which ensures that the initial wave vanishes near the boundaries and the interface. This initial wave setting is applied throughout the domain at the beginning time. For the later on, all values of electric and magnetic fields are computed based on the data of the previous time. In the present study, all four boundaries of the domain are assumed to be PEC [45].

For this example, we demonstrate the second and fourth order convergences. In our computations, we choose the number of time steps and the stop time to be $N_t = 10000$ and $t = 60$ ps, respectively. A reference solution is generated by the MIBTD4 with a dense grid ($N_x = 6401$ and $N_y = 51$). Note that one does not need to use a fine grid for the $y$
direction, since the wave solution is infinitely smooth in this direction. We thus set $N_y = 51$ and $M_y = 4$ in all computations, which are enough to resolve the Gaussian wave for our purpose and save the CPU time. The same higher order finite difference approximation with $N_y = 51$ and $M_y = 4$ is also used in the FDTD discretization of (4.1.1)–(4.1.4) along $y$ direction. Thus, the present FDTD is slightly different from that for the Example 1. For this reason, the present finite difference discretization will be simply termed as FD2.

The maximal errors of the MIBTD and FD2 methods by considering different $N = N_x$ values are depicted in Fig. 4.10. As in the Example 1, a linear least-squares fitting in log-log scale is conducted in all cases. The convergence rate of the FD2 method is found to be 1.30, which is better than the previous example. This may be because of the use of higher order finite difference approximations in the $y$ direction. Based on the same stencil bandwidth, the full second order is recovered by the MIBTD2 method with $r = 2.04$. For the MIBTD4, the overall order is $r = 4.25$. Thus, a fourth order of convergence is numerically achieved in the present 2D example.

**Figure 4.10:** Numerical convergence tests of $E_z$ for the Example 2 of the straight interface case in the Debye dispersive interface problems.
4.3.1.3 Example 3: Gaussian-Sine initial wave

We finally consider an example with a different initial condition. The same domain dimensions and Debye coefficients as in the Example 2 are considered, but the initial wave is chosen as

$$E_z(x, y, 0) = \exp\left(-\frac{(x - x_c)^2}{(2\alpha^2)}\right) \sin\left(\frac{4\pi y}{(d - c)}\right),$$

where $x_c$ and $\alpha$ are unchanged. For the left and right boundaries of the domain, the PEC condition [45] is assumed again, because the initial solution vanishes near these boundaries. For the top and bottom boundaries, the initial solution is chosen such that it equals to zero exactly on the boundaries. So, the PEC condition can also be imposed. Because the solution is oscillatory in the $y$ direction, a larger number of grid nodes $N_y = 101$ is employed. As before, $N_y = 101$ and $M_y = 4$ are fixed in all numerical tests, including the MIBTD and FD2 methods. Through the similar convergence tests, the convergence rate for the FD2,
MIBTD2, and MIBTD4 is found to be, respectively, $r = 1.36$, $r = 2.10$, and $r = 4.32$, see Fig. 4.12.

4.3.2 Curved interfaces

This section validates the proposed matched interface and boundary time-domain (MIBTD) method by considering dispersive curved-interface problems with constant curvature, non-constant curvatures, and sharp corners. In all studies, a uniform mesh is employed for the $E_z$ component, in which the numbers of grid points in both $x$ and $y$ directions are the same, i.e., $N_x = N_y$. For simplicity, we denote $N = N_x = N_y$. The staggered grids for $H_x$ and $H_y$ can then be correspondingly formed.

4.3.2.1 Dispersive Case 1a: Circular dispersive interface with a constant magnetic permeability

In our first dispersive case, we study a circular interface problem with magnetic permeability $\mu$ being chosen as $\mu_0$ through out the domain, i.e., $\mu^+ = \mu^- = \mu_0$. The domain dimensions are chosen as $[0 \text{ mm}, 30 \text{ mm}]^2$, and the interface $\Gamma$ of the Dispersive Case 1 is
defined to be
\[ \Gamma : \sqrt{(x - 6\pi)^2 + (y - 15)^2} = \frac{30}{7}, \] (4.3.1)
where the unit is also in millimeters. The circular cylinder is assumed to be a water medium with the Debye parameters: \( \epsilon_s = 81, \epsilon_\infty = 1.8, \) and \( \gamma = 9.4 \) ps \([6, 19]\). An incident pulse of the form \( E_z(x, y, t) = \exp(-(x + 15 - c_0 t)^2/(2\alpha^2)) \) is imposed as the boundary condition at the left boundary \( x = 0 \) mm. Here \( \alpha = 2.5 \) mm and \( c_0 \) is the speed of light in air. The computation will stop before the propagating wave hits the right boundary \( x = 30 \) mm and the scattered wave touches the top boundary \( y = 30 \) mm and bottom boundary \( y = 0 \) mm. So, for simplicity, the incident plane waves will be imposed on the top and bottom boundaries as well, while the perfectly electric conducting (PEC) boundary condition (see Section 2.6) is assumed on the right boundary.

The proposed second order MIBTD method is employed to solve the Maxwell-Debye system (4.2.30) for this circular dispersive interface problem. For a comparison, a FDTD discretization is also considered for (4.2.30). In particular, this FDTD algorithm shares the same spatial and temporal discretizations with the MIBTD method, except for the MIB interface treatment. The same boundary implementations [46] are utilized in both the MIBTD and FDTD approaches. In all cases, the stop time is always assigned as \( T = 110 \) ps which is short enough such that both the propagating and scattered waves have not reached the boundaries. In the present tests, we choose the mesh size \( N \) to be odd integers. This is because that there are no analytical solutions available for the dispersive interface problems. Thus, for the purpose of benchmarking our numerical results, a reference solution is generated by employing the second order MIBTD with a very dense grid \( N = 3201 \) and a sufficiently small \( \Delta t \). In our convergence analysis, in order to make sure that the numerical values on a coarse grid are also sampled in the reference solution, the mesh size \( N \) can only be chosen as some special odd integers. In particular, the necessary requirement for a tested mesh size \( N \) is that \( N - 1 \) is an integer factor of 3200. For example, when \( N = 401 \), the reference solution needs to be downsampled with a rate 8, i.e., keeping one \( E_z \) value in
Table 4.1: Critical CFL number $C$ for the circular Debye-dispersive interface problem in the TM mode with $\mu^- = \mu_0$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FDTD</th>
<th>MIBTD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Critical $N_t$</td>
<td>$C$</td>
</tr>
<tr>
<td>101</td>
<td>171</td>
<td>0.9151</td>
</tr>
<tr>
<td>201</td>
<td>215</td>
<td>1.4539</td>
</tr>
<tr>
<td>401</td>
<td>434</td>
<td>1.4371</td>
</tr>
<tr>
<td>801</td>
<td>873</td>
<td>1.4272</td>
</tr>
</tbody>
</table>

every eight $E_z$ values. The downsampled reference solution can then be compared with the numerical solution to compute the maximal error for $E_z$. We note that since the $H_x$ and $H_y$ nodes are staggered to the $E_z$ nodes, the present convergence analysis is not applicable to $H_x$ and $H_y$.

We first examine the stability of the dispersive MIBTD and FDTD algorithms. The CFL stability condition is also given by (3.3.8). For the present dispersive interface problem with dimension units, the maximum velocity $v_{\text{max}}$ equals to the speed of light in air, i.e., $v_{\text{max}} = c_0 = 3 \times 10^8$ m/s. Thus, the CFL condition can be rewritten as

$$\Delta t = C \frac{\Delta x}{c_0 \sqrt{2}},$$

(4.3.2)

where $\Delta t = 110 \times 10^{-12}/(N_t-1)$ in seconds and $\Delta x = 30 \times 10^{-3}/(N-1)$ in meters. Again, the value of the CFL constant $C$ is determined by both the spatial and temporal discretizations. Similarly, we numerically detect the critical $N_t$ value for a given $N$ value. The critical values and corresponding CFL numbers of the MIBTD and FDTD methods are listed in Table 4.1. These CFL results are very similar to those of the nondispersive case given in Table 3.1. In particular, we also have that as $\Delta x$ approaches to zero, the CFL number $C$ of the FDTD method goes to $C = \sqrt{2}$, while that of the MIBTD method is a constant within the interval $C \in [1.21, 1.26]$. For the FDTD results, this is can be explained by the fact that the same spatial and temporal discretizations are employed in the FDTD algorithm for both the nondispersive and dispersive interface problems. Nevertheless, we note that the one-sided
Table 4.2: Numerical convergence test of the circular Debye-dispersive interface problem in the TM mode with $\mu^- = \mu_0$ in the $L_{\infty}$ norm.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FDTD</th>
<th>MIBTD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Error</td>
<td>Order</td>
</tr>
<tr>
<td>321</td>
<td>2.60e-3</td>
<td></td>
</tr>
<tr>
<td>401</td>
<td>2.70e-3</td>
<td>-0.17</td>
</tr>
<tr>
<td>641</td>
<td>1.06e-3</td>
<td>1.99</td>
</tr>
<tr>
<td>801</td>
<td>1.10e-3</td>
<td>-0.17</td>
</tr>
</tbody>
</table>

Figure 4.13: Numerical convergence tests for the circular Debye-dispersive interface problem in the TM mode with $\mu^- = \mu_0$. Here, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.

Finite difference approximations underlying the MIB treatments for $H_x$ and $H_y$ are essentially the same as those for $E_z$. More specifically, we can characterize these approximations by a parameter $L$, which is the number of grid nodes (excluding the fictitious node) being used in each jump condition discretization. It is known that the stability of the MIB scheme mainly depends on this parameter $L$ [46]. Here, we have $L = 2$ for not only $H_x$ and $H_y$, but also $E_z$. Thus, the dispersive MIBTD algorithm attains the same CFL number as the nondispersive MIBTD method.

We next study the convergence rates of the dispersive MIBTD and FDTD algorithms. To ensure the stability, we take the CFL constant to be $C = 0.7$ in both methods. The $L_{\infty}$ errors in $E_z$ of the dispersive FDTD and MIBTD methods are listed in Table 4.2. As
Figure 4.14: The MIBTD solution with $N = 321$ at $t = 110$ ps for the circular Debye-dispersive interface problem in the TM mode with $\mu^- = \mu_0$. (a) Contour plot of $E_z$. (b) $E_z(x,15)$. (c) Contour plot of $H_y$. (d) $H_y(x,15)$. (e) Contour plot of $H_x$. (f) $H_x(17.06,y)$. 

95
Table 4.3: CPU time in seconds of the FDTD method ($T_F$) and the MIBTD method ($T_M$) for the Debye-dispersive circular interface problem in the TM mode with $\mu^- = \mu_0$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>CPU time of FDTD ($T_F$)</th>
<th>CPU time of MIBTD ($T_M$)</th>
<th>$T_M/T_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>1.95</td>
<td>4.31</td>
<td>2.21</td>
</tr>
<tr>
<td>161</td>
<td>8.13</td>
<td>20.80</td>
<td>2.56</td>
</tr>
<tr>
<td>201</td>
<td>15.83</td>
<td>35.94</td>
<td>2.27</td>
</tr>
<tr>
<td>321</td>
<td>67.27</td>
<td>143.50</td>
<td>2.13</td>
</tr>
<tr>
<td>401</td>
<td>141.97</td>
<td>285.67</td>
<td>2.01</td>
</tr>
<tr>
<td>641</td>
<td>551.73</td>
<td>1241.13</td>
<td>2.25</td>
</tr>
<tr>
<td>801</td>
<td>1000.19</td>
<td>2378.66</td>
<td>2.38</td>
</tr>
</tbody>
</table>

mentioned above, the errors are calculated against the reference solution. So, the mesh size $N$ cannot be arbitrarily chosen. On the other hand, in order to obtain reasonably accurate results for the FDTD algorithm, $N$ cannot be too small. Thus, we choose $N = 321$, 401, 641 and 801 in the present study. It can be seen that with these mesh refinements, the convergence of the FDTD method is not monotonic, perhaps because that $\Delta x$ is not halved in the mesh refinements. The least squares fitting is a good tool to identify the overall numerical order in such a situation. To this end, the FDTD errors are plotted in Fig. 4.13. The fitted convergence rate of the FDTD method is found to be $s = 1.16$. This justifies that the FDTD method degrades to a first order method, due to the lack of proper interface treatments. However, the MIBTD method attains a second order convergence after enforcing jump conditions for $H_x$, $H_y$ and $E_z$ across the dispersive interface, as can be seen in both Table 4.2 and Fig. 4.13. The contour plots and slice plots of the MIBTD solutions are shown in Fig. 4.14. The slices plots obviously reveal that the $E_z$ is $C^1$ continuous across the interface but $H_y$ and $H_x$ are only $C^0$.

Finally, we investigate the speed of the dispersive MIBTD method. The CPU times in seconds consumed in the FDTD and MIBTD computations are presented in Table 4.3. Here, we also take the CFL constant to be $C = 0.7$ in both approaches. As one may expected, the MIBTD method spends more time than the FDTD method for the present dispersive problem. We are more interested in the CPU time ratio of the MIBTD over the FDTD. It
Table 4.4: Critical CFL number $C$ for the circular Debye-dispersive interface problem in the TM mode with $\mu^- = 2\mu_0$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FDTD</th>
<th>MIBTD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_t$</td>
<td>$C$</td>
</tr>
<tr>
<td>101</td>
<td>171</td>
<td>0.9151</td>
</tr>
<tr>
<td>201</td>
<td>215</td>
<td>1.4539</td>
</tr>
<tr>
<td>401</td>
<td>434</td>
<td>1.4371</td>
</tr>
<tr>
<td>801</td>
<td>874</td>
<td>1.4229</td>
</tr>
</tbody>
</table>

Table 4.5: Numerical convergence test of the circular Debye-dispersive interface problem in the TM mode in the $L_\infty$ norm with $\mu^- = 2\mu_0$.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FDTD</th>
<th>MIBTD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Error</td>
<td>Order</td>
</tr>
<tr>
<td>321</td>
<td>9.89e-3</td>
<td></td>
</tr>
<tr>
<td>401</td>
<td>1.05e-2</td>
<td>-0.27</td>
</tr>
<tr>
<td>641</td>
<td>5.79e-3</td>
<td>1.27</td>
</tr>
<tr>
<td>801</td>
<td>4.44e-3</td>
<td>1.20</td>
</tr>
</tbody>
</table>

can be observed from Table 4.3 that this ratio is about 2.3 for a large $N$ value. However, if a high precision is required, the MIBTD algorithm is actually more cost-efficient. For example, if one needs to achieve an accuracy level of $1.00e - 3$, it can be seen in Table 4.2 that a dense mesh with $N = 801$ has to be used in the FDTD method, while a coarse mesh with $N = 321$ is sufficient for the MIBTD method. Referring to their CPU times in Table 4.3, the MIBTD method is obviously much faster.

4.3.2.2 Dispersive Case 1b: Circular dispersive interface with a piecewise constant magnetic permeability

In this case, the same material, domain and discretization parameters are chosen as in the previous dispersive case except the magnetic permeability value. To illustrate the effectiveness of proposed MIBTD method in handling discontinuous solutions, we set the $\mu$ value in the dispersive medium to be $2\mu_0$, i.e., $\mu^+ = \mu_0$ and $\mu^- = 2\mu_0$. It is noted that our dispersive material now becomes nonphysical.

Similar to the previous dispersive case, the numerical CFL numbers and convergence
results are reported in Table 4.4 and Table 4.5 respectively. We note that the numerical CFL numbers of this case are almost identical to the ones in the previous dispersive case, even though the present MIBTD algorithm becomes more involved. This is because we also choose $L = 2$ in the MIB discretization of mixed jump conditions. The convergence results of the MIBTD method for this case are not uniform at smaller grid sizes but the second order accuracy are still achieved at larger grid sizes. Fig. 4.15 plots the errors of both FDTD and MIBTD methods. It can be read from the Fig. 4.15 that the fitted convergence rate of FDTD method is $s = 0.96$. However the MIBTD method still successfully attains the second order convergence with $s = 2.14$ due to the use of the proper treatments at the interface.

We conclude this subsection by plotting the numerical solutions of electric and magnetic fields. Fig. 4.16 shows that in the present case, $E_z$ is still continuous across the interface, whereas $H_x$ and $H_y$ are both discontinuous across the interface.

4.3.2.3 Dispersive Case 2: complex dispersive interfaces

In the second case of dispersive interface problems, we study arbitrarily curved interfaces with nonconstant curvatures. For simplicity, the magnetic coefficient $\mu$ will be chosen as a
Figure 4.16: The MIBTD solution with $N = 321$ at $t = 110$ ps for the circular Deybe-dispersive interface problem in the TM mode with $\mu^- = 2\mu_0$. (a) Contour plot of $E_z$. (b) $E_z(x, 19.22)$. (c) Contour plot of $H_y$. (d) $H_y(x, 19.22)$. (e) Contour plot of $H_x$. (f) $H_x(15.66, y)$. 
constant $\mu = \mu_0$ throughout the domain in the rest of this paper. A family of interfaces parameterized by the polar angle $\theta$ [34] are studied in the Dispersive Case 2

$$\Gamma : \sqrt{(x - 6\pi)^2 + (y - 15)^2} = \frac{30}{t} + b \sin(m\theta), \quad \theta \in [0, 2\pi]. \quad (4.3.3)$$

The unit of this equation is in millimeters and so is that of the parameter $b$. Here the parameter $m$ determines the number of leaves of the core region and $b$ controls the magnitude of the curvature. Four independent tests with parameters $(m, b) = (2, 5/2), (3, 10/9), (4, 10/9)$ and $(5, 10/11)$ are considered as the Dispersive Case 2(a), 2(b), 2(c) and 2(d), respectively. The other problem settings including the domain dimensions, the Debye parameters, the incident wave, and boundary conditions, are the same as in the previous dispersive case. A stop time $T = 110$ ps is also employed. The results on the stability and execution time are similar to the circular dispersive interface case, and will not be presented here to save space. Essentially, the same CFL stability condition holds for the MIBTD algorithm, while the ratio of the CPU time costed by the MIBTD over that by the FDTD is also about 2.3.

**Table 4.6:** Numerical convergence tests of the complex Debye-dispersive interface cases for the TM mode in the $L_\infty$ norm.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Case 2(a) $(m = 2, b = 5/2)$</th>
<th>Case 2(b) $(m = 3, b = 10/9)$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD</td>
<td>MIBTD</td>
</tr>
<tr>
<td></td>
<td>Error Order</td>
<td>Error Order</td>
</tr>
<tr>
<td>101</td>
<td>1.68e-2</td>
<td>1.29e-2</td>
</tr>
<tr>
<td>161</td>
<td>1.08e-3 0.95</td>
<td>5.30e-3 1.91</td>
</tr>
<tr>
<td>201</td>
<td>7.40e-3 1.70</td>
<td>3.00e-3 2.56</td>
</tr>
<tr>
<td>321</td>
<td>4.20e-3 1.21</td>
<td>1.20e-3 1.96</td>
</tr>
<tr>
<td>101</td>
<td>2.80e-2</td>
<td>1.20e-2</td>
</tr>
<tr>
<td>161</td>
<td>1.15e-2 1.90</td>
<td>4.30e-3 2.30</td>
</tr>
<tr>
<td>201</td>
<td>9.40e-3 0.91</td>
<td>2.70e-3 2.10</td>
</tr>
<tr>
<td>321</td>
<td>6.10e-3 0.92</td>
<td>9.86e-4 2.15</td>
</tr>
</tbody>
</table>

We mainly focus on the impact of the arbitrarily curved interface on the accuracy of
Figure 4.17: Numerical convergence tests for the complex Debye-dispersive interface problems in the TM mode. Case 2(a): \((m, b) = (2, \frac{5}{2})\); Case 2(b): \((m, b) = (3, \frac{10}{9})\); Case 2(c): \((m, b) = (4, \frac{10}{9})\); Case 2(d): \((m, b) = (5, \frac{10}{11})\). In all charts, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.

the MIBTD method for this example. For each dispersive case, a reference solution is first generated by the MIBTD algorithm with \(N = 1601\) and a sufficiently small \(\Delta t\). By taking the CFL number to be \(C = 0.7\), the MIBTD and FDTD solutions based on several \(N\) values are compared with the reference solution on mutually sampled grid nodes. The calculated \(L_\infty\) errors in \(E_z\) are given in Table 4.6. It can be seen that the numerical order of the dispersive FDTD method is quite inconsistent. It sometimes becomes as large as 2.22, while sometimes is as low as 0.38. On the contrary, the numerical order for the MIBTD algorithm is always about 2 throughout the table. These errors are also analyzed in Fig. 4.17. As in the previous studies, a linear least-squares fitting is conducted in all cases. In particular,
it can be seen from Figures 4.18, 4.19, 4.20, and 4.21 that $E_z$ is $C^1$ continuous across the interface, but $H_y$ and $H_x$ are only $C^0$ continuous. Due to the loss of regularities in wave solutions near the interface, the convergence rates of the FDTD method are always found to be around first order. Specifically, the FDTD method delivers $s = 1.21$ for case 2(a), $s = 1.27$ for case 2(b), $s = 1.29$ for case 2(c), and $s = 1.30$ for case 2(d). However, by using the MIBTD method, the full second order is recovered in every case. In the present study, the numerical order $s$ of this method is found to be $s = 2.06$ for case 2(a), $s = 2.01$ for case 2(b), $s = 2.14$ for case 2(c), and $s = 2.04$ for case 2(d).

4.3.2.4 Dispersive Case 3: sharp dispersive interface

In the last case of dispersive interface problems, we study a Lipschitz continuous but not $C^1$ continuous interface. Once again, the constant magnetic permeability $\mu_0$ is employed. We define a $3/4$ circle interface parameterized by an angle $\theta$ as follows

\[ \Gamma : (x, y) = \begin{cases} 
(6\pi + \frac{30}{7} \cos \theta, 15 + \frac{30}{7} \sin \theta), & \text{if } 0 \leq \theta \leq \frac{3\pi}{4} \text{ or } \frac{5\pi}{4} \leq \theta \leq 2\pi, \\
(6\pi - \frac{60\sqrt{2}}{7} \left(1 - \frac{\theta}{\pi}\right), 15 + \frac{60\sqrt{2}}{7} \left(1 - \frac{\theta}{\pi}\right)), & \text{if } \frac{3\pi}{4} \leq \theta \leq \pi, \\
(6\pi + \frac{60\sqrt{2}}{7} \left(1 - \frac{\theta}{\pi}\right), 15 + \frac{60\sqrt{2}}{7} \left(1 - \frac{\theta}{\pi}\right)), & \text{if } \pi \leq \theta \leq \frac{5\pi}{4}.
\end{cases} \tag{4.3.4} \]

The unit of this equation is in millimeters. The other problem settings are the same as in the previous dispersive cases. A stop time $T = 110$ ps is also employed. The double layer MIB scheme needs to be applied to treat two sharp corners on the edge of the incomplete circle. For other irregular points, the regular MIB scheme can be used. The impact of the double layer MIB scheme on the stability and execution time of the MIBTD algorithm is negligible. In particular, it is found that the same CFL stability condition holds for the MIBTD algorithm, while the ratio of the CPU time costed by the MIBTD over that by the
Figure 4.18: The MIBTD solution with $N = 321$ at $t = 110$ ps for the Debye-dispersive Case 2(a) with parameters $(b, m) = (2, 5/2)$ in the TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 12)$. (c) Contour plot of $H_y$. (d) $H_y(x, 12)$. (e) Contour plot of $H_x$. (f) $H_x(15, y)$. 


Figure 4.19: The MIBTD solution with $N = 321$ at $t = 110$ ps for the Debye-dispersive Case 2(b) with parameters $(b, m) = (3, 10/9)$ in the TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 10.78)$. (c) Contour plot of $H_y$. (d) $H_y(x, 10.78)$. (e) Contour plot of $H_x$. (f) $H_x(15, y)$. 
Figure 4.20: The MIBTD solution with $N = 321$ at $t = 110$ ps for the Debye-dispersive Case 2(c) with parameters $(b, m) = (4, 10/9)$ in the TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 19.22)$. (c) Contour plot of $H_y$. (d) $H_y(x, 19.22)$. (e) Contour plot of $H_x$. (f) $H_x(16.88, y)$. 
Figure 4.21: The MIBTD solution with $N = 321$ at $t = 110$ ps for the Debye-dispersive Case 2(d) with parameters $(b, m) = (5, 10/11)$ in the TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 11.06)$. (c) Contour plot of $H_y$. (d) $H_y(x, 11.06)$. (e) Contour plot of $H_x$. (f) $H_x(16.4, y)$. 
Table 4.7: Numerical convergence test of the sharp Debye-dispersive interface case in the $L_\infty$ norm for the TM mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Error</th>
<th>Order</th>
<th>Error</th>
<th>Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>201</td>
<td>5.80e-3</td>
<td></td>
<td>1.33e-2</td>
<td></td>
</tr>
<tr>
<td>321</td>
<td>1.67e-2</td>
<td>-2.26</td>
<td>2.60e-3</td>
<td>3.49</td>
</tr>
<tr>
<td>401</td>
<td>5.90e-3</td>
<td>4.68</td>
<td>1.00e-3</td>
<td>4.29</td>
</tr>
<tr>
<td>801</td>
<td>1.40e-3</td>
<td>2.08</td>
<td>4.08e-4</td>
<td>1.30</td>
</tr>
</tbody>
</table>

FDTD is also about 2.3.

From the accuracy point of view, the double layer MIB scheme is indispensable for the present sharp dispersive interface. Without the double layer scheme, there are a few irregular nodes near the sharp corners, for which one cannot generate the necessary fictitious points for them. If neglecting these irregular nodes, the accuracy of the MIBTD algorithm would be essentially the same as that of the FDTD method. Nevertheless, after applying the double layer MIB interface treatment, the full second order can be secured throughout the domain. To illustrate this, we first generate a reference solution by the MIBTD algorithm with $N = 1601$ and a sufficiently small $\Delta t$. By taking the CFL number to be $C = 0.7$, the $L_\infty$ errors in $E_z$ for the MIBTD and FDTD solutions are reported in Table 4.7 and plotted in Fig. 4.22. It can be seen that the order of the MIBTD is not uniform, while that of the

Figure 4.22: Numerical convergence tests for the sharp Debye-dispersive interface case in the TM mode. Here, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.
FDTD even becomes negative in one refinement. This may be due to the presence of the corner points. In fact, it can be observed in the contour plots and slice plots shown in Fig. 4.23 that the solutions, particularly two magnetic components, exhibit some nearly singular behavior near two corner points. It is thus amazing to see that the overall convergence rate of the MIBTD method is 2.49 for this tough problem. This validates the effectiveness of the MIB double layer treatment and the accuracy of the entire MIBTD algorithm.

4.4 Conclusion

In the present study, we generalize the previous matched interface and boundary time domain (MIBTD) method [6] designed for 1D problem to deal with straight, curved and/or sharp dispersive interfaces of Debye type in solving two-dimensional transverse magnetic system with both electric and magnetic coefficients being discontinuous. Based on the auxiliary differential equation approach, a hybrid Maxwell-Debye system is constructed, which couples the wave equation for the electric component with Maxwell’s equations for the magnetic components. This allows us to track the transient changes in the regularities of electromagnetic fields across the dispersive interfaces. The resulting time dependent jump conditions are rigorously enforced through regular and double layer interface treatments. Numerical results demonstrate that for both arbitrarily curved interfaces and interfaces with sharp corners, and for both continuous and discontinuous electromagnetic fields, the proposed MIBTD method can fully recover the second order of accuracy, while the classical finite difference time domain (FDTD) method yields only the first order of accuracy. The stability condition of the MIBTD method has a slightly smaller stability constant than that of the FDTD method. For a given grid, the execution time of the MIBTD method is about 2.3 times of that of the FDTD method. However, if one aims to achieve a certain accuracy level, the MIBTD method requires a much coarse grid, so that the MIBTD method is actually more cost-efficient.

In comparing with the previously developed matched interface and boundary (MIB)
Figure 4.23: The MIBTD solution with $N = 321$ at $t = 110$ ps for the sharp Debye-dispersive interface in the TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 11.72)$. (c) Contour plot of $H_y$. (d) $H_y(x, 11.72)$. (e) Contour plot of $H_x$. (f) $H_x(16.86, y)$. 
schemes for solving Maxwell’s equations in the time domain [6, 26], Chapter 3 and the Helmholtz equation in the frequency domain [34], the present MIB algorithms have three major new features:

1. In this work, a curved interface problem based on the staggered Yee lattice has been treated for the first time in the MIB literature. In the previous MIB schemes for elliptic and Helmholtz problems with curved interfaces [34], only non-staggered meshes have been studied. Although the staggered meshes have been considered in the previous MIB schemes for Maxwell’s equations [6, 26], only straight interface problems are involved in these studies. The straight interface greatly simplifies the numerical implementation, because the MIB interface treatment needs to be carried out only at one interface location and can be applied to other locations directly. However, the present development of MIB interface treatments for arbitrary interfaces with electric and magnetic components defined at different nodes becomes much more complicated, because the treatments at different interface locations and for different field components are all different. This general approach allows ones to directly obtain the jump conditions for the straight interfaces. This feature emphasizes the flexibility of our proposed method. A sophisticated code has to be written to implement such a MIB algorithm.

2. The MIB sharp interface treatment is implemented for the first time for solving computational electromagnetic (CEM) interface problems in this work. The double layer MIB scheme was originally developed in [57] for elliptic interface problems, and has never been applied to the CEM problems. With this enhancement, the proposed MIB algorithm really can handle very complicated and $C^0$ continuous interfaces.

3. Though the MIBTD method reported in Chapter 3 is able to handle the discontinuous electromagnetic wave solutions. However, the waves’ regularities for that case only time-independent. The method in this present work has to take care of the time-
dependent jump conditions by introducing the interface auxiliary equations (IADEs). These ODEs permit the track of the transient changes in the regularity along the interface. As a result, a very sophisticated MIB scheme is developed in this chapter successfully secure up to the 6th order accurate for the straight interfaces and a second order accurate for curved interface FDTD simulation. This is a significant accomplishment in the development of the MIB methods for solving CEM interface problems.
Chapter 5

TIME-DOMAIN MATCHED INTERFACE AND BOUNDARY METHODS FOR DRUDE
DISPERSSIVE INTERFACE PROBLEMS IN TM MODE

5.1 Introduction

In Chapter 4, we introduced a novel MIBTD method for the dispersive interface problems. Based on numerous numerical results, that new algorithm is very robust and achieves high order accuracy for different shapes of the interfaces. However, the previous MIBTD development only focused on Debye materials. Additional issues need to be addressed in extending it to the Drude materials. In particular, the auxiliary differential equation (ADE) of the Drude material is a second order differential equation while that of the Debye medium is just first order. We note that the Drude model may be decomposed into a linear combination of a Debye model and a constant-conductivity model, so that only first order ADEs need to be solved numerically. However, such an approach involves not only electromagnet fields, but also the current density. This introduces grand difficulty to the MIBTD modeling, because the jump conditions of the current density are generally unknown. A second order ADE model for the Drude material is thus more tractable to the MIBTD method, in which jump conditions are only enforced for electric and magnetic fields. To the authors’ knowledge, no high order interface treatment has ever been developed to deal with the second order Drude materials in the FDTD literature. This chapter is based on our published work [9].

The Drude model is used to simulate the movement of the electron in the solids, i.e. conduction. In the mathematical model, the constitutive relations of the single-order Drude model is already derived by using ADE approach in (2.3.7). Therefore, the Drude-Maxwell
system for the TM\textsubscript{z} mode is fully written as
\begin{align}
\frac{\partial H_x}{\partial t} &= -\frac{1}{\mu_0} \frac{\partial E_z}{\partial y}, \quad (5.1.1) \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu_0} \frac{\partial E_z}{\partial x}, \quad (5.1.2) \\
\frac{\partial D_z}{\partial t} &= \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}, \quad (5.1.3) \\
\frac{\partial^2 D_z}{\partial t^2} + \gamma \frac{\partial D_z}{\partial t} &= \epsilon_0 \epsilon_\infty \frac{\partial^2 E_z}{\partial t^2} + \epsilon_0 \epsilon_\infty \gamma \frac{\partial E_z}{\partial t} + \epsilon_0 \omega_1^2 E_z. \quad (5.1.4)
\end{align}

Motivated by interface considerations, we propose a new Maxwell-Drude system
\begin{align}
\frac{\partial E_z}{\partial t} &= \dot{E}_z, \quad \frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \frac{\partial E_z}{\partial x}, \quad \frac{\partial H_x}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_z}{\partial y}, \\
\frac{\partial \dot{E}_z}{\partial t} &= -\gamma \dot{E}_z - \frac{\omega_1^2}{\epsilon_\infty} E_z + \frac{1}{\mu_0 \epsilon_0 \epsilon_\infty} \left( \frac{\partial^2 E_z}{\partial x^2} + \frac{\partial^2 E_z}{\partial y^2} \right) + \frac{\gamma}{\epsilon_0 \epsilon_\infty} \left( \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} \right). \quad (5.1.5)
\end{align}

Obviously, this new system is a hybrid one coupling the first order equations for \(H_x\) and \(H_y\) with the wave equation for \(E_z\). Its equivalence to the classical Maxwell-Drude system can be easily established within a homogeneous Drude material. For an inhomogeneous problem involving a dispersive interface, physical interface conditions must be satisfied in the numerical discretization. We note that three Drude parameters \(\epsilon_\infty, \omega_1,\) and \(\gamma\) could be discontinuous across the dispersive interface.

### 5.2 Interface jump conditions

A typical Drude interface problem will be studied in this paper. Consider a 2D domain of a rectangle shape \(\Omega = [a, b] \times [c, d]\). Assume that an interface \(\Gamma\) separates the domain \(\Omega\) into two parts \(\Omega^+\) and \(\Omega^-\), where \(\Gamma\) could be either a straight line or a curve. For two media on both hand sides of \(\Gamma\), if one of them is a Drude medium, we will refer to \(\Gamma\) as a Drude interface. For simplicity, we will assume the other medium, say \(\Omega^+\), being the air or vacuum.
in the present study. Define the jump of a function \( u(x, y) \) at \( \Gamma \) to be \( [u] := u^+ - u^- \), where the superscript, \(-\) or \(+\), denotes the limiting value of function from one side or from the other side of the interface. For the present Drude-air dispersive interface, we assume the material equation (2.2.5) in the vacuum \( \Omega^+ \) as well with \( \varepsilon_\infty^+ = 1 \) and \( \omega_1^+ = 0 \). Then, the high frequency limit \( \varepsilon_\infty \) and the Drude pole frequency \( \omega_1 \) in (5.1.4) are both discontinuous across the interface \( \Gamma \). Here, \( \gamma^+ \) is a free parameter so that we can assume \( \gamma = \gamma^- = \gamma^+ \) being a constant throughout \( \Omega \).

Across the interface \( \Gamma \), jump conditions for field components are imposed based on (2.6.1) as follows

\[
\vec{n} \times (E^+ - E^-) = 0, \quad \vec{n} \cdot (D^+ - D^-) = 0,
\]

\[
\vec{n} \times (H^+ - H^-) = 0, \quad \vec{n} \cdot (\mu H^+ - \mu H^-) = 0,
\]

(5.2.1)

where \( \vec{n} \) is the unit vector normal to the interface, pointing from \( \Omega^- \) into \( \Omega^+ \). Denote \( \vec{\tau} \) as the tangential direction at an interface point. A local Cartesian coordinate \((\vec{n}, \vec{\tau}, \vec{z})\) can then be assumed at this interface point. Consequently, six zeroth order jump conditions can be derived from (5.2.1)

\[
[E_z] = 0, \quad [E_\tau] = 0, \quad [D_n] = 0, \quad [H_z] = 0, \quad [H_\tau] = 0, \quad [H_n] = 0.
\]

(5.2.2)

As in [6, 26] and Chapter 4, these zeroth order jump conditions will be combined with Maxwell’s equations to derive the first order jump conditions for both electric and magnetic components

\[
\left[ \frac{\partial E_z}{\partial n} \right] = 0, \quad \left[ \frac{\partial E_\tau}{\partial \tau} \right] = 0, \quad \left[ \frac{\partial H_\tau}{\partial \tau} \right] = 0, \quad \left[ \frac{\partial H_n}{\partial n} \right] = 0, \quad \left[ \frac{\partial H_n}{\partial n} \right] = 0.
\]

(5.2.3)

We still need one more first order jump condition. Following [6] and Chapter 4, let us suppose that \( [\partial D_z/\partial t] = \psi(t, x, y) \) for some unknown function \( \psi(t, x, y) \). We then take the
jump operation to the equation (5.1.3) to deduce the last jump condition

\[ \psi(t, x, y) = \left[ \frac{\partial D_z}{\partial t} \right] = \left[ \frac{\partial H_y}{\partial x} \right] - \left[ \frac{\partial H_x}{\partial y} \right]. \]  

(5.2.4)

Since the field components are Cartesian ones in (5.1.5), we need to transfer the jump conditions (5.2.2) and (5.2.3) into the Cartesian coordinate as in Chapter 4. Denote the angle between \( \vec{n} \) and the \( x \)-axis as \( \theta \). Then the field components in the local coordinate and the Cartesian coordinate are related via simple coordinate transformations, i.e., \( H_n = \cos \theta H_x + \sin \theta H_y \) and \( H_\tau = -\sin \theta H_x + \cos \theta H_y \). It is easy to derive the following zeroth order jump conditions

\[ [H_x] = 0, \quad [H_y] = 0, \quad [E_z] = 0. \]  

(5.2.5)

The first order jump conditions can be found by using the coordinate transformation for derivative operator (3.2.5) For two conditions of \( E_z \) given in (5.2.3), the coordinate rotation gives

\[ \left[ \frac{\partial E_z}{\partial x} \right] = 0, \quad \left[ \frac{\partial E_z}{\partial y} \right] = 0. \]  

(5.2.6)

In combining these two conditions with the continuity condition of \( E_z \) given in (5.2.5), we thus have three Cartesian conditions for \( E_z \), which can be handled by the previous MIB method in Chapter 4. Similarly, we apply the coordinate transformation to other three conditions in (5.2.3). This gives rise to

\[
0 = \left[ \frac{\partial H_n}{\partial n} \right] = \cos^2 \theta \left[ \frac{\partial H_x}{\partial x} \right] + \cos \theta \sin \theta \left[ \frac{\partial H_x}{\partial y} \right] + \sin \theta \cos \theta \left[ \frac{\partial H_y}{\partial x} \right] + \sin^2 \theta \left[ \frac{\partial H_y}{\partial y} \right], \\
0 = \left[ \frac{\partial H_\tau}{\partial \tau} \right] = \sin^2 \theta \left[ \frac{\partial H_x}{\partial x} \right] - \cos \theta \sin \theta \left[ \frac{\partial H_x}{\partial y} \right] - \sin \theta \cos \theta \left[ \frac{\partial H_y}{\partial x} \right] + \cos^2 \theta \left[ \frac{\partial H_y}{\partial y} \right], \\
0 = \left[ \frac{\partial H_n}{\partial \tau} \right] = -\sin \theta \cos \theta \left[ \frac{\partial H_x}{\partial x} \right] + \cos^2 \theta \left[ \frac{\partial H_y}{\partial x} \right] - \sin^2 \theta \left[ \frac{\partial H_y}{\partial y} \right] + \cos \theta \sin \theta \left[ \frac{\partial H_y}{\partial y} \right].
\]

By solving these three equations together with (5.2.4), we attain the desired Cartesian jump
conditions for $H_x$ and $H_y$

\[
\begin{bmatrix}
\frac{\partial H_y}{\partial x} \\
\frac{\partial H_x}{\partial y}
\end{bmatrix} = \psi(t, x, y) \cos^2 \theta, \\
\begin{bmatrix}
\frac{\partial H_y}{\partial x} \\
\frac{\partial H_x}{\partial y}
\end{bmatrix} = -\psi(t, x, y) \sin^2 \theta.
\]  

(5.2.7)

We note that for a straight interface case with $\theta = 0$, (5.2.7) can be further simplified.

The nonhomogeneous terms in (5.2.7) are unknown and time dependent. Thus, in the computation, one needs to estimate $\psi(t, x, y)$ at interface points at each time step. In order to calculate such values, we apply jump operators to (5.1.4) to derive the following interface auxiliary differential equation (IADE)

\[
\frac{\partial \psi(t, x, y)}{\partial t} + \gamma \psi(t, x, y) = \epsilon_0 \left[ \epsilon_\infty \frac{\partial \dot{E}_z}{\partial t} \right] + \epsilon_0 \gamma \left[ \epsilon_\infty \dot{E}_z \right] + \epsilon_0 \left[ \omega^2 E_z \right],
\]  

(5.2.8)

We note that the proposed IADE (5.2.8) for the Drude material is a second order differential equation, while that of the Debye material is a first order one (see (2.3.4)). A new difficulty here is how to approximate the highest order term, i.e., $\frac{\partial \dot{E}_z}{\partial t}$, in the MIBTD algorithm.

We first simplify the right hand side term of (5.2.8). Thanks to the continuity of $E_z$ and its time derivatives across $\Gamma$, this term can be rewritten as

\[
g(t, x, y) := \epsilon_0 \left[ \epsilon_\infty \frac{\partial \dot{E}_z}{\partial t} \right] + \epsilon_0 \gamma \left[ \epsilon_\infty \dot{E}_z \right] + \epsilon_0 \left[ \omega^2 E_z \right] \\
= \epsilon_0 (\epsilon_\infty^+ - \epsilon_\infty^-) \left( \frac{\partial \dot{E}_z}{\partial t} \right)^+ + \epsilon_0 \gamma (\epsilon_\infty^+ - \epsilon_\infty^-) \dot{E}_z^+ + \epsilon_0 (\omega_1^+)^2 - (\omega_1^-)^2 E_z^+.
\]  

(5.2.9)

Here we have introduced a new notation for $g(t, x, y)$, so that (5.2.8) can be denoted as

\[
\frac{\partial \psi(t, x, y)}{\partial t} + \gamma \psi(t, x, y) = g(t, x, y).
\]  

(5.2.10)

Equation (5.2.9) suggests that $g(t, x, y)$ can be evaluated based on $E_z$, $\dot{E}_z$ and $\frac{\partial \dot{E}_z}{\partial t}$ values from the positive side. The details of such an evaluation procedure will be offered in next section. Here, the positive side is chosen in the present study, because the incident wave
propagates from the positive domain $\Omega^+$. Alternatively, we can also use $\dot{E}_z$ and $E_z^-$ to estimate $g(t, x, y)$, if necessary. With the approximated $g(t, x, y)$ value, (5.2.10) enables us to calculate $\psi(t, x, y)$ at various interface points at each time step. We thus are able to track the unsteady nonhomogeneous values of (5.2.7), so that all Cartesian jump conditions become deterministic. Finally, we note that it is because we need to know values of $\dot{E}_z$ in (5.2.9) that we propose the new Maxwell-Drude system (5.1.5), instead of employing the classical TM Eqs. (5.1.1) to (5.1.4).

### 5.3 MIB time domain algorithm

The present Drude interface problem consists of the proposed Maxwell-Drude system (5.1.5) and the IADE (5.2.10). The boundary conditions on the interface $\Gamma$ are given by (5.2.5), (5.2.6), and (5.2.7), while some proper boundary conditions will be assumed on the $\partial \Omega$.

In the present study, the classical fourth order Runge-Kutta method (Section 2.4.3) is employed to integrate both the Maxwell-Drude system (5.1.5) and the IADE (5.2.10) with a fixed time increment $\Delta t$. Because each fractional step of the four stage Runge-Kutta time integration can be regarded as an Euler integration [40], we will illustrate the proposed MIBTD algorithm by considering a simple forward Euler time-stepping from $t_k$ to $t_{k+1}$ for simplicity.

A uniform staggered grid shown in Fig. 4.2 is used in our computations. Without the loss of generality, we assume that the interface $\Gamma$ will not pass any grid point in the present work. Since the geometry is time invariant, we can determine all necessary interface points $(x_o, y_o)$, which are the intersection points between $\Gamma$ and $x$ grid lines or $y$ grid lines, at the beginning of computation. In the following discussion, without the loss of generality, we assume that at the time $t_k$, we know field values of $E_z$, $H_x$, and $H_y$ on staggered nodes and interface values of $\psi(t_k, x_o, y_o)$ on interface points.

In the MIBTD algorithm presented in Section 4.2.4, away from the interface, the standard
finite difference discretization of (5.1.5) is conducted, while for staggered nodes near $\Gamma$, the MIB interface treatment will be carried out to correct finite difference approximations via imposing the jump conditions.

After correcting all finite difference approximations by the MIB scheme, the spatial discretization of the Maxwell-Drude system (5.1.5) is ensured to be second order of accuracy at time $t_k$. One can then integrate (5.1.5) to next time level $t_{k+1}$ to generate new values of $E_z$, $H_x$, and $H_y$. We will update the IADE (5.2.10) from $t_k$ to $t_{k+1}$ as well. For this purpose, we shall calculate $g(t_k, x_o, y_o)$ at the interface point $(x_o, y_o)$ first. To overcome the aforementioned difficulty due to the involvement $\frac{\partial E_z}{\partial t}$ in the IADE, we propose to reformulate the expression of $g(t, x, y)$ by substituting the last equation of (5.1.5) into (5.2.9)

$$g(t_k, x_o, y_o) = \left[ \frac{\epsilon_0 \epsilon_{\infty} (\omega_1^+)^2 - \epsilon_0 (\omega_1^-)^2}{\epsilon_{\infty}^+} \right] E_z^+$$

so that the explicit calculation of $\frac{\partial E_z}{\partial t}$ is not required. Nevertheless, one needs to evaluate various derivative and function values at the off-grid point $(x_o, y_o)$ in (5.3.1). Fortunately, the MIB scheme is a robust finite difference method, which allows these values being approximated by using on-grid function values exclusively from the positive side. For example, $(\partial^2 E_z^+ / \partial x^2)(t_k, x_o, y_o)$ will be approximated via one-sided interpolation based on several nearby derivative values of $(\partial^2 E_z^+ / \partial x^2)(t_k, x_i, y_j)$ for some $i$ and $j$. Then $(\partial^2 E_z^+ / \partial x^2)(t_k, x_i, y_j)$ can be approximated by finite differences using $E_z^+$ values within $\Omega^+$. Other terms in (5.3.1) can be similarly treated. With $g(t_k, x_o, y_o)$ values, we integrate the IADE (5.2.10) in time to generate interface values $\psi(t_{k+1}, x_o, y_o)$, which will be used in the MIB scheme for next time level $t_{k+1}$. This completes one time step of the proposed MIBTD algorithm.

It is noted that for a straight interface case, the jump conditions can be iteratively enforced (Section 4.2.4.1) so that high order MIBTD algorithms can be easily constructed. It is also noted that most computations of the MIB jump condition enforcement need to
be conducted only once at the beginning, because the geometric domain, grid, and spatial
discretization of the jump conditions are all time invariant. The calculated representation
coefficients that express the fictitious values in terms of field values will be re-used in all
time steps.

5.4 Numerical Experiments

In this section, we investigate the accuracy and stability of the proposed MIBTD algo-

rithm for solving straight and curved interface problems. Different types of curved interfaces
with constant curvature, fluctuating curvature and sharp corner are studied. In all studies,
a uniform mesh is employed for the $E_z$ component, in which the number of grid points in
both $x$ and $y$ directions is denoted, respectively, as $N_x$ and $N_y$. The staggered grids for $H_x$
and $H_y$ can then be correspondingly formed. By setting the initial wave solutions as trivially
zero at $t = 0$, numerical time integration is carried out for $N_t$ steps, until a stopping time
$T$. Here the time increment is given as $\Delta t = T/N_t$. Numerical errors in the $L_\infty$ norm will
be reported in all examples.

5.4.1 Example 1: Straight Drude interface

We first consider a straight interface problem, for which the MIBTD algorithm can be
easily generalized to higher order. In this example, the computational domain is considered as
$\Omega = [0 \mu m, 3 \mu m]^2$ with the interface $\Gamma$ located at $x = 0.75\pi \mu m$. A dispersive gold medium is
placed on the right subdomain $\Omega^-$ with the Drude parameters $\epsilon_\infty = 9.84$, $\omega_1 = 9.096$ eV, and
$\gamma = 0.072$ eV [58, 59]. An incident pulse of the form $E_z(x, y, t) = \exp(-(x+1.5-c_0 t)^2/(2\alpha^2))$
is enforced as the boundary condition at the left boundary $x = 0 \mu m$. Here $\alpha = 0.075 \mu m$
and $c_0$ is the speed of light in air. We note that both the media and the incident wave are
invariant along the $y$ direction, so that the electromagnetic wave solutions to this straight
interface problem will be constant along the $y$ direction. Therefore, periodic conditions
will be assumed on the top boundary $y = 3 \mu m$ and the bottom boundary $y = 0 \mu m$ for
simplicity. As in Section 4.3.1, our simulation will stop before the transmitted wave hits the right boundary \( x = 3 \, \mu\text{m} \). Under this assumption, we can impose the perfectly electric conducting (PEC) boundary condition (Section 2.6) at \( x = 3 \, \mu\text{m} \) for simplicity.

Higher order MIBTD schemes are examined for this example. Following Section 4.3.1, away from the interface, the standard \((2M)\)th order central finite difference approximation will be carried out in both \( x \) and \( y \) directions. Here \( M \) is the half stencil bandwidth. Near the interface, the zeroth and first order jump conditions will be discretized by using \( 2L \) function values and \( 2 \) fictitious values at the first step, where one-sided approximations involving \( L \) grid nodes in one side are used to ensure the sufficiently high accuracy. One can then iteratively enforce these two jump conditions, until a total of \( 2M \) fictitious values are solved [26, 34]. Then, the \((2M)\)th order central finite difference can be conducted across the interface. Three MIBTD schemes are considered, i.e., the MIBTD2 with \((M, L) = (1, 2)\), the MIBTD4 with \((M, L) = (2, 4)\), and the MIBTD6 with \((M, L) = (3, 6)\). Theoretically, these three schemes attain second, fourth, and sixth order of accuracy, respectively. The approximation in the \( y \) direction is not critical in this example, because the wave solutions are trivially constant along this direction. Thus, we will take \( N_y = 10 \) in all tests and consider different \( N_x \) values. For a comparison, a FDTD method is considered in this paper which discretizes the Maxwell-Drude system (5.1.5) by the central finite difference in space and the classical fourth order Runge-Kutta method in time. Computationally, this FDTD method is simply attained by switching off the MIB fictitious value representation in the MIBTD2 scheme.

We first qualitatively benchmark the MIBTD algorithm by studying the wideband reflection coefficient of an air-gold interface. The MIBTD2 scheme is employed with \( N_x = 1601 \). Two time series are recorded for the \( E_z \) values at two fixed observation points in the vacuum with a time increment \( \Delta t = 0.0027 \, \text{fs} \) and a total of 10,000 time steps. Through proper processing, one can generate the incident and reflected pulses based on the recorded time series. The numerical reflection coefficient can then be calculated as the ratio of the discrete
Figure 5.1: Numerical results of Example 1 for a straight air-gold interface in TM mode. (a) The reflection coefficient at a straight air-gold interface; (b) Numerical convergence test.

Table 5.1: Critical CFL number $C$ for Example 1 for Drude-dispersive interface in TM mode. Here $N_t^*$ denotes the critical $N_t$ value.

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>FDTD</th>
<th>MIBTD2</th>
<th>MIBTD4</th>
<th>MIBTD6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_t^*$</td>
<td>$C$</td>
<td>$N_t^*$</td>
<td>$C$</td>
</tr>
<tr>
<td>101</td>
<td>91</td>
<td>1.4587</td>
<td>91</td>
<td>1.4587</td>
</tr>
<tr>
<td>201</td>
<td>182</td>
<td>1.4543</td>
<td>182</td>
<td>1.4543</td>
</tr>
<tr>
<td>401</td>
<td>365</td>
<td>1.4492</td>
<td>365</td>
<td>1.4492</td>
</tr>
<tr>
<td>801</td>
<td>739</td>
<td>1.4313</td>
<td>739</td>
<td>1.4313</td>
</tr>
</tbody>
</table>

Fourier transformation of the reflected and incident pulses. Fig. 5.1 (a) compares the magnitude of the reflection coefficient as a function of frequency to the analytical one. It can be seen that the MIBTD result and the exact one are in good agreement over a wide range of frequencies. This validates the proposed MIBTD algorithm.

We next investigate the stability of the proposed MIBTD method. For the stability study, a stopping time $T = 13.23$ fs is used, which is short enough such that both reflected and transmitted pulses have not reached the horizontal boundaries. The Courant-Friedrichs-Lewy (CFL) stability condition for solving Maxwell’s equations in 2D is known to be (Section 2.5.5)

$$
\Delta t \leq C \frac{1}{v_{\max} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}. \quad (5.4.1)
$$
Here, we have that $\Delta x$ is different from $\Delta y$ and the maximum velocity $v_{\text{max}}$ equals to the speed of light in air, i.e., $v_{\text{max}} = c_0 = 3 \times 10^8$ m/s. The CFL constant $C$ is determined by both the spatial and temporal discretizations. We note that because the present FDTD approach is based on the fourth order Runge-Kutta method, instead of the Leapfrog scheme, the present CFL constant $C$ differs from the one of the standard FDTD scheme by a factor of $\sqrt{2}$ (Section 2.5.5).

In order to examine the stability of the proposed algorithms, we numerically detect the critical $N_t$ value for each scheme. Here, the critical $N_t$ value is defined in the sense that a even smaller $N_t$ value will render the computation to be unstable. In particular, for a given $N_x$ value, we examine all possible $N_t$ values. For a particular $N_t$ value, say $N_t^*$, such that the final $L_\infty$ error is less than a tolerance, e.g. 1, the computation is said to be stable. If the final error of $N_t^* - 1$ is greater than or equal to the tolerance, the empirical critical $N_t$ value is taken as $N_t^*$. By considering several $N_x$ values, the critical $N_t$ values and the corresponding CFL constants for both the FDTD and MIBTD methods are reported in Table 5.1. It can be seen that as $\Delta x$ becomes smaller and smaller, the CFL number $C$ of the present FDTD method goes to $C = \sqrt{2}$. In fact, $C = \sqrt{2}$ is the analytical CFL number of the present FDTD method (Section 2.5.5). This validates the present numerical procedure for the stability analysis. For the proposed MIBTD algorithms, no analytical result is available. We thus numerically explore the CFL number $C$ for different MIBTD schemes. It can be seen from Table 5.1 that the MIBTD2 scheme attains the same CFL number as the FDTD. In other words, the MIB interface treatment in the MIBTD2 has negligible impact on the stability for this straight interface problem. For the MIBTD4 and MIBTD6, $C$ decreases as $M$ is larger as expected, because $C$ is known to be inversely proportional to the absolute sum of the underlying finite difference weights [26].

We then quantitatively examine the accuracy of the proposed higher order MIBTD methods. We conduct a numerical convergence analysis by considering different spatial size $N_x$ while $N_y$ is always fixed to be 10. To ensure the stability, we take the CFL constant to
Table 5.2: Numerical convergence test of Example 1 for Drude-dispersive interface in TM mode.

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>FDTD</th>
<th>MIBTD2</th>
<th>MIBTD4</th>
<th>MIBTD6</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Error</td>
<td>Order</td>
<td>Error</td>
<td>Order</td>
</tr>
<tr>
<td>201</td>
<td>1.07E-1</td>
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<td>1.45E-2</td>
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<tr>
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<td>4.12E-2</td>
<td>1.38</td>
<td>1.33E-2</td>
<td>2.28</td>
</tr>
<tr>
<td>801</td>
<td>1.39E-2</td>
<td>1.57</td>
<td>3.00E-3</td>
<td>2.15</td>
</tr>
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<td>1601</td>
<td>6.10E-3</td>
<td>1.19</td>
<td>8.36E-4</td>
<td>1.84</td>
</tr>
</tbody>
</table>

be $C = 0.7$ in all methods. Because there is no analytical solution available for this Drude interface problem, we benchmark our numerical results by considering a numerical reference solution. This reference solution is generated by considering the most accurate MIBTD6 scheme with a very dense grid $N_x = 12801$ and a sufficiently small $\Delta t$. Based on this reference solution, the $L_\infty$ errors in the $E_z$ component are reported in Table 5.2. The numerical orders calculated based on two successive meshes are also reported. The orders of three MIBTD schemes are indeed about two, four, and six, respectively. Without the interface treatment, the FDTD scheme is obviously degraded to the first order of accuracy. For a visual comparison, the $L_\infty$ errors in Table 5.2 are also plotted in Fig. 5.1 (b). A linear least-squares fitting [34] is conducted in the log-log scale for the purpose of determining the overall convergence rate $r$ of the scheme. Here the fitted convergence lines are shown as solid lines in Fig. 5.1 (b) with $r$ being the slopes. The averaged orders of both MIBTD and FDTD methods are close to the theoretical estimates.

Fig. 5.2 presents the slice of $E_z$ and $H_y$ generated by MIBTD6 method. Plot of $H_x$ is lacking due to the trivial solution. It can be seen that $E_z$ is $C^1$ continuous across the interface but $H_y$ is only $C^0$.

We finally investigate the computational speed of the MIBTD methods. The CPU time in seconds of both the FDTD and MIBTD methods are listed in Table 5.3. All computations here are conducted on an SGI Xeon E5-4640 CPU core operating at 2.4 GHZ and 8 GB of memory. As in the numerical convergence tests, the CFL constant is set to be $C = 0.7$. It is seen in Table 5.3 that the CPU time of the MIBTD methods becomes larger when the
Figure 5.2: The MIBTD6 solution with $N_x = 401$, $N_y = 10$ at $t = 13.23$ fs of Example 1 for Drude-dispersive interface in TM mode. (a) $E_z(x, 1.5)$. (b) $H_y(x, 1.5)$.

Table 5.3: CPU time in seconds of the FDTD method ($T_F$), the MIBTD2 method ($T_{M2}$), the MIBTD4 method ($T_{M4}$) and the MIBTD6 method ($T_{M6}$) for Example 1 for Drude-dispersive interface in TM mode.

<table>
<thead>
<tr>
<th>$N_x$</th>
<th>FDTD $T_F$</th>
<th>MIBTD2 $T_{M2}$</th>
<th>$T_{M2}/T_F$</th>
<th>MIBTD4 $T_{M4}$</th>
<th>$T_{M4}/T_F$</th>
<th>MIBTD6 $T_{M6}$</th>
<th>$T_{M6}/T_F$</th>
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<td>0.368</td>
<td>3.54</td>
<td>0.468</td>
<td>4.50</td>
</tr>
<tr>
<td>401</td>
<td>0.410</td>
<td>0.576</td>
<td>1.40</td>
<td>0.780</td>
<td>1.90</td>
<td>1.720</td>
<td>4.20</td>
</tr>
<tr>
<td>801</td>
<td>1.620</td>
<td>1.952</td>
<td>1.20</td>
<td>2.412</td>
<td>1.49</td>
<td>3.320</td>
<td>2.05</td>
</tr>
<tr>
<td>1601</td>
<td>6.460</td>
<td>6.550</td>
<td>1.01</td>
<td>7.284</td>
<td>1.13</td>
<td>9.200</td>
<td>1.42</td>
</tr>
</tbody>
</table>

order is higher. The ratio of the CPU time of the MIBTD over that of the FDTD is also listed in Table 5.3. This ratio becomes much smaller when $N_x$ is larger. This is because
the generation of fictitious value representation needs to be carried out only once in the MIB scheme. Thus, the additional CPU time caused by the MIB treatment becomes less significant comparing with the overall CPU time used in the Runge-Kutta time integrations, when \( N_x \) is larger. Therefore, the ratio of the MIBTD2 over the FDTD eventually goes to 1.01 when \( N_x \) is very large, while that between the MIBTD6 and FDTD is about 1.42. Even though the MIBTD methods consume more CPU time than the FDTD, the MIBTD methods are actually more cost-efficient. When one aims to achieve certain high precision, the MIBTD method based on a coarser grid is actually much faster.

5.4.2 Example 2: Circular Drude interface

We next study a circular Drude interface problem with \( \Gamma \) defined as

\[
\Gamma : \sqrt{(x - 0.7\pi)^2 + (y - 1.75)^2} = 0.5, \tag{5.4.2}
\]

where the unit is in micrometers. The entire domain \( \Omega = [0 \mu m, 3.5 \mu m]^2 \) consists of two subdomains. The subdomain \( \Omega^- \) inside the cylinder is assigned to be a dispersive gold medium with the same Drude parameters as in Example 1. The subdomain \( \Omega^+ \) is assumed to be air. An incident pulse of the form \( E_z(x,y,t) = \exp(-(x + 1.75 - c_0t)^2/(2\alpha^2)) \) is imposed as the boundary condition at the left boundary \( x = 0 \mu m \) with \( \alpha = 0.25 \mu m \). The computation will be terminated before the propagating wave hits the right boundary \( x = 3.5 \mu m \) and the scattered wave touches the top boundary \( y = 3.5 \mu m \) and bottom boundary \( y = 0 \mu m \). For these reasons, the stopping time is chosen as \( T = 13.40 \) fs. Moreover, for simplicity, the top and bottom boundary conditions are enforced according to the incident pulses, while the PEC boundary condition (Section 2.6) is imposed on the right boundary.

For curved Drude interface problems, the generalization of the MIBTD algorithm to higher order is not straightforward. Thus, only the second order MIBTD2 scheme will be considered in the curved interface problems, and this scheme is simply referred to as the
Critical CFL number $C$ for Example 2 for Drude-dispersive interface in TM mode. Here $N_t^*$ denotes the critical $N_t$ value.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FDTD</th>
<th></th>
<th>MIBTD</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>102</td>
<td>1.5914</td>
<td>112</td>
<td>1.4493</td>
</tr>
<tr>
<td>201</td>
<td>219</td>
<td>1.5481</td>
<td>236</td>
<td>1.3756</td>
</tr>
<tr>
<td>401</td>
<td>450</td>
<td>1.4428</td>
<td>508</td>
<td>1.2781</td>
</tr>
<tr>
<td>801</td>
<td>907</td>
<td>1.4317</td>
<td>1052</td>
<td>1.2344</td>
</tr>
</tbody>
</table>

Numerical convergence test of Example 2 for Drude-dispersive interface in TM mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>FDTD</th>
<th></th>
<th>MIBTD</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>4.12e-2</td>
<td></td>
<td>1.57e-2</td>
<td></td>
</tr>
<tr>
<td>201</td>
<td>1.85e-2</td>
<td>1.16</td>
<td>4.60e-3</td>
<td>1.77</td>
</tr>
<tr>
<td>401</td>
<td>7.30e-3</td>
<td>1.34</td>
<td>1.00e-3</td>
<td>2.20</td>
</tr>
<tr>
<td>801</td>
<td>3.90e-3</td>
<td>0.90</td>
<td>2.28e-4</td>
<td>2.13</td>
</tr>
</tbody>
</table>

We next examine the numerical orders of the MIBTD and FDTD methods. A numerical reference solution is generated by the MIBTD scheme with a dense mesh $N = 1601$. Maximum errors calculated with respect to this reference solution are reported in Table 5.5 and...
Figure 5.3: Numerical convergence test of Example 2 for Drude-dispersive interface in TM mode. Here, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.

Table 5.6: CPU time in seconds of the FDTD method ($T_F$) and the MIBTD method ($T_M$) for Example 2 for Drude-dispersive interface in TM mode.

<table>
<thead>
<tr>
<th>N</th>
<th>$T_F$</th>
<th>$T_M$</th>
<th>$T_M/T_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>0.37</td>
<td>0.43</td>
<td>1.16</td>
</tr>
<tr>
<td>201</td>
<td>3.00</td>
<td>3.40</td>
<td>1.13</td>
</tr>
<tr>
<td>401</td>
<td>26.99</td>
<td>34.93</td>
<td>1.29</td>
</tr>
<tr>
<td>801</td>
<td>247.80</td>
<td>334.42</td>
<td>1.35</td>
</tr>
</tbody>
</table>

also plotted in Fig. 5.3. The contour plots and slice plots of MIBTD solution are shown in Fig. 5.4. A sharp change is clearly seen across the interface $\Gamma$ in the $H_y$ and $H_x$ components. In general, we know that $E_z$ is $C^1$ continuous across $\Gamma$, while the regularity of $H_y$ and $H_x$ degrades to $C^0$. Without proper interface treatment, the staircase error is severe in the FDTD algorithm. Thus, the least-squares fitted convergence rate of the FDTD method is found to be 1.15 for the present example. However, the MIBTD method still successfully retains the second order convergence after enforcing jump conditions for $H_x, H_y$ and $E_z$ across the interface.

Our final test for the present example is again exploring the speed of MIBTD method. The CPU time in seconds consumed by the FDTD and MIBTD methods is reported in Table
Figure 5.4: The MIBTD solution with $N_x = N_y = 401$ at $t = 13.40$ fs for Example 2 for Drude-dispersive interface in TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 1.75)$. (c) Contour plot of $H_y$. (d) $H_y(x, 1.75)$. (e) Contour plot of $H_x$. (f) $H_x(2.0, y)$. 
5.6. Because in the curved interface case, different MIB treatments have to be conducted at different irregular points, the computational overhead of the MIB scheme becomes larger than that of the straight interface case. Thus, the CPU time ratio of the MIBTD method over the FDTD method in the present study is about 1.35 when \( N \) is large. Nevertheless, we note that the MIBTD method is still more cost-efficient than the FDTD method.

5.4.3 Example 3: Complex Drude interfaces

We next examine the robustness of the MIBTD algorithm in dealing with complex interfaces with non-constant curvatures. A family of interfaces parameterized by the polar angle \( \theta \) [34] are studied for this purpose

\[
\Gamma : \sqrt{(x - 0.7\pi)^2 + (y - 1.75)^2} = 0.5 + b \sin(m\theta), \quad \theta \in [0, 2\pi]. \tag{5.4.4}
\]

The unit of this equation as well as \( b \) is in micrometers. Here the parameter \( m \) determines the number of leaves of the core region and \( b \) controls the magnitude of the curvature. As in [8], we investigate four independent cases: Case 1, \((m, b) = (2, 1/4)\); Case 2, \((m, b) = (3, 1/9)\); Case 3, \((m, b) = (4, 1/9)\); Case 4, \((m, b) = (5, 1/11)\). Apart from the difference in the definition of the interface, the other problem settings including the domain dimensions, Drude parameters, incident wave, boundary conditions and stopping time are the same as in Example 2.

The stability and CPU behaviors of the MIBTD and FDTD methods are similar to those of Example 2, and thus are not presented here to save space. We only focus on the accuracy of the MIBTD method in solving various non-constant curvature interfaces. In order to benchmark the numerical convergences, for each case, a reference solution is generated by the MIBTD algorithm with \( N = 1601 \) and a sufficiently small \( \Delta t \). We again set the CFL number to be \( C = 0.7 \). The MIBTD and FDTD solutions based on different \( N \) values are compared with the reference solution on mutually sampled grid nodes. The
Table 5.7: Numerical convergence tests of Example 3 for Drude-dispersive interface in TM mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Case 1, $(m, b) = (2, 1/4)$</th>
<th></th>
<th>Case 2, $(m, b) = (3, 1/9)$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD</td>
<td>MIBTD</td>
<td>FDTD</td>
<td>MIBTD</td>
</tr>
<tr>
<td></td>
<td>Error</td>
<td>Order</td>
<td>Error</td>
<td>Order</td>
</tr>
<tr>
<td>101</td>
<td>6.00E-2</td>
<td>2.00E-2</td>
<td>6.04E-2</td>
<td>2.16E-2</td>
</tr>
<tr>
<td>201</td>
<td>2.94E-2</td>
<td>1.03</td>
<td>5.80E-3</td>
<td>1.79</td>
</tr>
<tr>
<td>401</td>
<td>1.47E-2</td>
<td>1.00</td>
<td>1.40E-3</td>
<td>2.05</td>
</tr>
<tr>
<td>801</td>
<td>6.80E-3</td>
<td>1.11</td>
<td>3.15E-4</td>
<td>2.15</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N$</th>
<th>Case 3, $(m, b) = (4, 1/9)$</th>
<th></th>
<th>Case 4, $(m, b) = (5, 1/11)$</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD</td>
<td>MIBTD</td>
<td>FDTD</td>
<td>MIBTD</td>
</tr>
<tr>
<td></td>
<td>Error</td>
<td>Order</td>
<td>Error</td>
<td>Order</td>
</tr>
<tr>
<td>101</td>
<td>4.33E-2</td>
<td>1.63E-2</td>
<td>6.94E-2</td>
<td>2.29E-2</td>
</tr>
<tr>
<td>201</td>
<td>2.37E-2</td>
<td>0.87</td>
<td>5.70E-3</td>
<td>1.52</td>
</tr>
<tr>
<td>401</td>
<td>9.40E-3</td>
<td>1.33</td>
<td>1.30E-3</td>
<td>2.13</td>
</tr>
<tr>
<td>801</td>
<td>4.20E-3</td>
<td>1.16</td>
<td>2.48E-4</td>
<td>2.39</td>
</tr>
</tbody>
</table>

results on maximum errors in $E_z$ are reported in Table 5.7. It can be seen that, the order convergences of the FDTD method always stay at around one, while those of the MIBTD algorithm are often about two throughout the table. Similar to the previous examples, the errors are also depicted in Fig 5.5, augmented by the linear least-squares fitting to analyze the numerical orders. Due to the loss of regularity in wave solutions near the interface, the convergence rates of the FDTD method are found to be $r = 1.15$, $r = 1.17$, $r = 1.14$ and $r = 1.27$, respectively, for the Case 1, 2, 3, and 4. After the MIB interface treatment, the accuracies of the MIBTD method are all about second order, even though the shape of the interface becomes more and more complicated. The present study demonstrates the robustness of the proposed MIBTD algorithm. Lastly, the contour and slice plots of the MIBTD solutions in four cases are shown in Figs. 5.6 to 5.9. A very complicated interaction between the electromagnetic waves and the Drude interface can be clearly seen, especially when the interface shape becomes more irregular.
Figure 5.5: Numerical convergence tests for Example 3 for Drude-dispersive interface in TM mode. Here, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines. (a) Case 1, \((m,b) = (2, 1/4)\); (b) Case 2, \((m,b) = (3, 1/9)\); (c) Case 3, \((m,b) = (4, 1/9)\); (d) Case 4, \((m,b) = (5, 1/11)\).

5.4.4 Example 4: Non-smooth Drude interface

In the previous examples, the interfaces are always \(C^1\) continuous, so that the regular MIB interface treatment is sufficient to treat them. In our last study, we consider a Lipschitz continuous but not \(C^1\) continuous interface to validate the proposed MIB non-smooth interface treatment. For this purpose, a 3/4 circle interface parameterized by the polar angle
Figure 5.6: The MIBTD solution with $N_x = N_y = 401$ at $t = 13.40$ fs for Example 3 for Drude-dispersive interface in TM mode case 1 with parameters $(m, b) = (2, 1/4)$. (a) Contour plot of $E_z$.  (b) $E_z(x, 1.4)$. (c) Contour plot of $H_y$.  (d) $H_y(x, 1.4)$. (e) Contour plot of $H_x$.  (f) $H_x(1.75, y)$. 

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Figure 5.7: The MIBTD solution with $N_x = N_y = 401$ at $t = 13.40$ fs for Example 3 for Drude-dispersive interface in TM mode case 2 with parameters $(m, b) = (3, 1/9)$. (a) Contour plot of $E_z$. (b) $E_z(x, 1.27)$. (c) Contour plot of $H_y$. (d) $H_y(x, 1.27)$. (e) Contour plot of $H_x$. (f) $H_x(1.75, y)$. 
Figure 5.8: The MIBTD solution with $N_x = N_y = 401$ at $t = 13.40$ fs for Example 3 for Drude-dispersive interface in TM mode case 3 with parameters $(m, b) = (4, 1/9)$. (a) Contour plot of $E_z$. (b) $E_z(x, 2.19)$. (c) Contour plot of $H_y$. (d) $H_y(x, 2.19)$. (e) Contour plot of $H_x$. (f) $H_x(1.95, y)$. 
Figure 5.9: The MIBTD solution with $N_x = N_y = 401$ at $t = 13.40$ fs for Example 3 for Drude-dispersive interface in TM mode case 4 with parameters $(m, b) = (5, 1/11)$. (a) Contour plot of $E_z$. (b) $E_z(x, 1.32)$. (c) Contour plot of $H_y$. (d) $H_y(x, 1.32)$. (e) Contour plot of $H_x$. (f) $H_x(1.88, y)$.
Table 5.8: Numerical convergence test of Example 4 for Drude-dispersive interface in TM mode.

<table>
<thead>
<tr>
<th>N</th>
<th>FDTD Error</th>
<th>FDTD Order</th>
<th>MIBTD Error</th>
<th>MIBTD Order</th>
</tr>
</thead>
<tbody>
<tr>
<td>201</td>
<td>2.10E-2</td>
<td></td>
<td>6.10E-3</td>
<td></td>
</tr>
<tr>
<td>321</td>
<td>2.23E-2</td>
<td>-0.13</td>
<td>5.70E-3</td>
<td>0.14</td>
</tr>
<tr>
<td>401</td>
<td>1.02E-2</td>
<td>3.52</td>
<td>2.70E-3</td>
<td>3.36</td>
</tr>
<tr>
<td>801</td>
<td>4.90E-3</td>
<td>1.06</td>
<td>2.90E-4</td>
<td>3.23</td>
</tr>
</tbody>
</table>

θ is defined as follows

\[
\Gamma : (x, y) = \begin{cases} 
(0.7\pi + 0.5 \cos \theta, \ 1.75 + 0.5 \sin \theta), & \text{if } 0 \leq \theta \leq \frac{3\pi}{4} \text{ or } \frac{5\pi}{4} \leq \theta \leq 2\pi, \\
(0.7\pi - \sqrt{2} \left(1 - \frac{\theta}{\pi}\right), \ 1.75 + \sqrt{2} \left(1 - \frac{\theta}{\pi}\right)), & \text{if } \frac{3\pi}{4} \leq \theta \leq \pi, \\
(0.7\pi + \sqrt{2} \left(1 - \frac{\theta}{\pi}\right), \ 1.75 + \sqrt{2} \left(1 - \frac{\theta}{\pi}\right)), & \text{if } \pi \leq \theta \leq \frac{5\pi}{4}.
\end{cases}
\] (5.4.5)

The unit of this equation is in micrometers. The other problem settings are the same as in the previous example. Due to appearances of two sharp corners on the left part of the interface Γ, the double layer MIB algorithm is indispensable. The CFL stability condition and execution time of the MIBTD algorithm remain essentially the same as in the previous curved interfaces. For this reason, those results are not presented here.

It is of interests to investigate the impact of the sharp corners on the accuracy of the MIBTD method. As usual, a reference solution is generated by the MIBTD scheme with \( N = 1601 \) and a sufficiently small \( \Delta t \). The CFL number is set to be \( C = 0.7 \) for all computations. The \( L_\infty \) errors involved in the MIBTD and FDTD \( E_z \) solutions are reported in Table 5.8 and plotted in Fig 5.10. These results reveal that the orders of both methods are highly nonuniform, due to the presence of the corner points. Indeed, the contour and slice plots given in Fig. 5.11 shows that the wave solutions display almost singular behavior near two corner points. The graphical least-squares analysis conducted in Fig. 5.10 gives a better estimate to the numerical orders than the tabulated results shown in Table 5.8. In particular, the numerical order of the FDTD and MIBTD is found to be 1.14 and 2.32,
Figure 5.10: Numerical convergence test of Example 4 for Drude-dispersive interface in TM mode. Here, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.

respectively. Without the double layer MIB scheme, the MIBTD algorithm will not be able to restore the fully second order of accuracy in solving only Lipschitz continuous interfaces.

5.5 Conclusion

In this Chapter, we propose a new Maxwell-Drude formulation for studying 2D transverse magnetic problems involving Drude materials with curved and non-smooth dispersive interfaces. This hybrid system couples the wave equation for the electric component with Maxwell’s equations for the magnetic components, and allows us to track the transient change in the regularity of electromagnetic fields across the Drude interfaces. The resulting time dependent jump conditions are enforced through regular and double layer interface treatments in the proposed MIBTD algorithm. For straight interfaces, the MIBTD method can be generalized to higher order, while for both curved interfaces and interfaces with sharp corners, the MIBTD method can fully recover the second order of accuracy. Thus, the proposed MIBTD method is more accurate and cost-efficient than the classical FDTD method.
Figure 5.11: The MIBTD solution with $N_x = N_y = 401$ at $t = 13.40$ fs of Example 4 for Drude-dispersive interface in TM mode. (a) Contour plot of $E_z$. (b) $E_z(x, 1.4)$.
(c) Contour plot of $H_y$. (d) $H_y(x, 1.4)$. (e) Contour plot of $H_x$. (f) $H_x(2.01, y)$. 
Chapter 6

TIME-DOMAIN MATCHED INTERFACE AND BOUNDARY METHODS FOR DEBYE DISPERSIVE INTERFACE PROBLEMS IN TE MODE

6.1 Introduction

In Chapter 4, we discussed the second-order MIBTD method for Debye media with complex interfaces in the TM mode. Unfortunately, that proposed scheme cannot be straightforwardly extended for the TE mode. That is because of the jump conditions of the electric field \( \mathbf{E} = (E_x, E_y, E_z) \). In the TM\(_z\) mode, \( E_z \) component is continuous throughout the domain. Even in the piecewise magnetic parameter case, the first order of \( E_z \) may not be trivial but still time-independent. For the TE\(_z\) mode with inhomogenous media, the zeroth and first order jump conditions of \( E_x \) and \( E_y \) need much attention since they are time dependent and are associated with the unknown flux density \( D_x \) and \( D_y \). As a result, new jump condition formulations have to be proposed. In addition, the standard Maxwell equations is taken into consideration instead of the hybrid Maxwell system because the flux density components are significant correlate of jump conditions' construction. Consequently, the leapfrog scheme is employed as the time-stepping scheme to simplified the discretizations of the time-dependent jump condition formulations. This Chapter is relied on our ongoing work [10].

By combining (2.1.21) and (2.3.4), one can obtain the Maxwell system for Debye disper-
sive media the in TE\textsubscript{z} mode as

\[
\frac{\partial D_x}{\partial t} = \frac{\partial H_z}{\partial y}, \quad (6.1.1)
\]

\[
\frac{\partial D_y}{\partial t} = -\frac{\partial H_z}{\partial x}, \quad (6.1.2)
\]

\[
\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left( \frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right), \quad (6.1.3)
\]

\[
D_x + \gamma \frac{\partial D_x}{\partial t} = \epsilon_0 \epsilon_s E_x + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t}, \quad (6.1.4)
\]

\[
D_y + \gamma \frac{\partial D_y}{\partial t} = \epsilon_0 \epsilon_s E_y + \gamma \epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t}. \quad (6.1.5)
\]

Notice that the Maxwell system (6.1.1)–(6.1.5) in the TE mode is quite more complex than
than its counter part in the TM mode (4.1.1)–(4.1.4) due to the appearances of two material
equations (6.1.4) and (6.1.5) instead of one. In addition, similar to the observation in the
TM mode case presented in Chapter 4, the material parameters \( \epsilon_s, \epsilon_\infty, \gamma \) and \( \mu \) can be
discontinuous along the material interface. Therefore, the emergence of Eqs. (6.1.4) and
(6.1.5) could significantly reduce the regularities of the electromagnetic fields across the
interface.

6.2 Matched and interface boundary (MIB) algorithm for TE mode

Similar to the MIBTD algorithm designed for the TM mode, jump conditions for the
proposed scheme for TE mode will be specified on the local coordinate system at first. Those
interface conditions shall be then formulated on the regular system to be effectively
incorporated in the MIB method.

6.2.1 Interface jump conditions in a local coordinate

The rectangle region \( \Omega \subseteq \mathbb{R}^2 \) is our computational domain. An interface \( \Gamma \) splits domain
\( \Omega \) into two subdomains \( \Omega^- \) and \( \Omega^+ \) as in Fig. 4.1.
It is analogous to the TM mode problem (see Chapter 4), the medium of each subdomain \( \Omega^+ \) and \( \Omega^- \) is assigned to be air and water respectively. A jump of a function value \( u \) across the interface \( \Gamma \) is defined as: \([u] = u^+ - u^-\), in which subscript +, or − refers to the limiting value from the corresponding side. By adopting that definition, the parameters in Debye model for the vacuum \( \Omega^+ \) are assigned to be \( \epsilon_+^s = \epsilon_\infty^+ = 1 \). The relaxation time \( \gamma \) for this dispersive interface problem is now a free parameter, so it can be constant throughout the domain \( \Omega \), i.e. \( \gamma^+ = \gamma^- = \gamma \). Therefore, across the interface \( \Gamma \), only permittivities at static frequency \( \epsilon_s \), at high frequency limit \( \epsilon_\infty \) are piecewise constant. In addition, for simplicity, magnetic permeability \( \mu \) is assumed to be invariant.

Across the interface \( \Gamma \), the jump conditions of field components in the TE mode follows the general ones described in (2.6.1), which yields

\[
\vec{n} \times (\vec{E}^+ - \vec{E}^-) = 0, \quad \vec{n} \cdot (\vec{D}^+ - \vec{D}^-) = 0, \quad \vec{n} \times (\vec{H}^+ - \vec{H}^-) = 0, \quad \vec{n} \cdot (\mu \vec{H}^+ - \mu \vec{H}^-) = 0,
\]

(6.2.1)

where \( \vec{n} \) is the unit vector normal to the interface, pointing from \( \Omega^- \) into \( \Omega^+ \). By following the similar approaches reported in Chapters 4 and 5, the interface conditions (6.2.1) will be expanded on a local coordinate illustrated in Fig. 4.1. Also, it is noted that the tangential derivative has no influence on the jump operator. The jump conditions (6.2.1) are then simplified on that local coordinate as follows

- For \( H \) components:

\[
[H_z] = 0, \quad [H_\tau] = 0, \quad [H_n] = 0, \quad \left[ \frac{\partial H_z}{\partial \tau} \right] = 0.
\]

(6.2.2)

- For \( E \) components:

\[
[E_\tau] = 0, \quad \left[ \frac{\partial E_\tau}{\partial \tau} \right] = 0.
\]

(6.2.3)
For $D$ components:

$$[D_n] = 0, \left[ \frac{\partial D_n}{\partial \tau} \right] = 0. \quad (6.2.4)$$

### 6.2.2 Interface jump conditions in the Cartesian coordinate system

According to (6.2.2), the zeroth jump condition for $H_z$ field is already determined as $[H_z] = 0$. To derive the next higher order jump conditions for this field, one takes the jump condition operator on Eqs. (6.1.1) and (6.1.2) to get

$$\left[ \frac{\partial D_x}{\partial t} \right] = \left[ \frac{\partial H_z}{\partial y} \right], \quad \left[ \frac{\partial D_y}{\partial t} \right] = -\left[ \frac{\partial H_z}{\partial x} \right]. \quad (6.2.5)$$

However, the jump conditions $\left[ \frac{\partial D_x}{\partial t} \right]$, and $\left[ \frac{\partial D_y}{\partial t} \right]$ are still unspecified.

Following (6.2.4), we have $[D_n] = 0$. Therefore, from the transformation (3.2.4), we obtain

$$[D_y] = [D_\tau] \cos \theta, \quad [D_x] = -[D_\tau] \sin \theta. \quad (6.2.6)$$

One then can take the time derivative of (6.2.6) to get the following relations

$$\left[ \frac{\partial D_y}{\partial t} \right] = \left[ \frac{\partial D_\tau}{\partial t} \right] \cos \theta, \quad \left[ \frac{\partial D_x}{\partial t} \right] = -\left[ \frac{\partial D_\tau}{\partial t} \right] \sin \theta. \quad (6.2.7)$$

The knowledge of the first order jump conditions for $D_x$ and $D_y$ will be fully achieved if the value of $[D_\tau]$ is defined. By that motivation, we formulate constitutive relations for Debye media (6.1.4)–(6.1.5) w.r.t the tangential direction in the local coordinate system

$$\gamma \frac{\partial D_\tau}{\partial t} + D_\tau = \epsilon_0 \epsilon_\infty \gamma \frac{\partial E_\tau}{\partial t} + \epsilon_0 \epsilon_s E_\tau. \quad (6.2.8)$$

We now take jump operators on both sides of (6.2.8), and keep in mind that $[E_\tau] = 0$ (due to (6.2.3)). By letting $\psi_{D_\tau}(t, x, y) = [D_\tau]$, and employing the coordinate transformation
(3.2.4), one attains

\[
\gamma \left[ \frac{\partial D_\tau}{\partial t} \right] + [D_\tau] = \epsilon_0 \gamma \left[ \epsilon_\infty \frac{\partial E_\tau}{\partial t} \right] + \epsilon_0 [\epsilon_s E_\tau] \tag{6.2.9}
\]

\[
\gamma \frac{\partial \psi_{D_\tau}}{\partial t} + \psi_{D_\tau} = \epsilon_0 \gamma \left( \epsilon_\infty^+ - \epsilon_\infty^- \right) \left( \frac{\partial E_\tau}{\partial t} \right)^+ + \epsilon_0 \left( \epsilon_s^+ - \epsilon_s^- \right) E_\tau^+ \tag{6.2.10}
\]

in which

\[
E_\tau^+ = -\sin \theta E_x^+ + \cos \theta E_y^+. \tag{6.2.11}
\]

It is noted that on-interface values of electric fields in the interface auxiliary differential equation (IADE) (6.2.10) are interpolated by nearby on-grid points from the positive direction in the general approach. In some cases, if the approximation from that direction is not applicable, the opposite interpolated path will be employed. This observation is also valid for our similar upcoming derivations. Furthermore, \([D_\tau]\) or \(\psi_{D_\tau}\) will be gained if one solves the above IADE (6.2.10). By adopting the relations (6.2.5) and (6.2.7), the first order jump conditions for the magnetic component \(H_z\) are expressed as follows

\[
\left[ \frac{\partial H_z}{\partial x} \right] = -\cos \theta \left[ \frac{\partial \psi_{D_\tau}}{\partial t} \right], \quad \left[ \frac{\partial H_z}{\partial y} \right] = -\sin \theta \left[ \frac{\partial \psi_{D_\tau}}{\partial t} \right]. \tag{6.2.12}
\]

Regarding the zeroth jump conditions of the electric fields, the interface condition (6.2.3) only gives us \([E_\tau] = 0\). Therefore, to completely establish the lowest order jump conditions for the electric components on the Cartesian grid, the information of \([E_n]\) is required. That quantity can be achieved by employing the constitutive relations of the Debye model. Specifically, one can rewrite the relations (6.1.4) and (6.1.5) along the normal direction, and then apply the jump operator to get

\[
\gamma \left[ \frac{\partial D_n}{\partial t} \right] + [D_n] = \epsilon_0 \gamma \left[ \epsilon_\infty \frac{\partial E_n}{\partial t} \right] + \epsilon_0 [\epsilon_s E_n]. \tag{6.2.13}
\]
The left hand side of (6.2.13) will be simplified to become zero on account of \([D_n] = 0\) (due to (6.2.4)). Meanwhile, the right hand side of (6.2.13) can be made simpler by letting \(\psi_{E_n}(t, x, y) = [E_n]\), and using the fact that \([\epsilon_\infty(\partial E_n/\partial t)] = (\epsilon_\infty^+ - \epsilon_\infty^-)(\partial E_n/\partial t)^+ + \epsilon_\infty^-(\partial \psi_{E_n}/\partial t)\), and \([\epsilon_s E_n] = (\epsilon_s^+ - \epsilon_s^-)E_n^+ + \epsilon_s^- \psi_{E_n}\). Finally, we end up with an IADE version of Eq. (6.2.13)

\[
\gamma \epsilon_\infty^- \frac{\partial \psi_{E_n}}{\partial t} = -\epsilon_s^- \psi_{E_n} - \gamma (\epsilon_\infty^+ - \epsilon_\infty^-) \left( \frac{\partial E_n}{\partial t} \right)^+ - (\epsilon_s^+ - \epsilon_s^-) E_n^+,
\]

(6.2.14)

where

\[
E_n^+ = \cos \theta E_x^+ + \sin \theta E_y^+.
\]

(6.2.15)

When the value of \([E_n] = \psi_{E_n}\) is available by solving the IADE (6.2.14), the zeroth jump conditions for electric components in the Cartesian system can be deduced by recalling \([E_r] = 0\), and employing local coordinate transformation (3.2.4)

\[
[E_x] = \cos \theta \psi_{E_n}, \quad [E_y] = \sin \theta \psi_{E_n}.
\]

(6.2.16)

The process of seeking for the first order jump conditions of electric components is more complicated than their counterpart. To construct these jump conditions in the Cartesian coordinate system, four linearly independent equations accepting \([\partial E_x/\partial x], [\partial E_y/\partial x], [\partial E_x/\partial y]\), and \([\partial E_y/\partial y]\) as variables are needed. One of such these equations can be derived from the first order interface condition in (6.2.3). Utilizing the derivative operator (3.2.5), one gets

\[
0 = \left[ \frac{\partial E_x}{\partial \tau} \right] = \sin^2 \theta \left[ \frac{\partial E_x}{\partial x} \right] - \sin \theta \cos \theta \left[ \frac{\partial E_y}{\partial x} \right] - \sin \theta \cos \theta \left[ \frac{\partial E_x}{\partial y} \right] + \cos^2 \theta \left[ \frac{\partial E_y}{\partial y} \right].
\]

(6.2.17)

Three equations left are unknown yet, but they can be found by exploiting Maxwell’s
equations, divergence free, and constitutive relations of the considered material. To begin
with, we apply jump operator on Eq. (6.1.3)

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

(6.2.18)

Since \( H_z \) and \( \mu \) are continuous across the interface, Eq. (6.2.18) can be further simplified as follows

\[
0 = \left[ \frac{\partial E_x}{\partial y} \right] - \left[ \frac{\partial E_y}{\partial x} \right].
\]  

(6.2.19)

To look for another equation regarding the first order jump conditions of \( E_x \) and \( E_y \), one can make a use of Gauss’ law for the electric field, and engage the property of the TE\(_z\) mode that material is invariant along the \( z \)-direction to attain

\[
\frac{\partial D_n}{\partial n} + \frac{\partial D_\tau}{\partial \tau} = 0.
\]  

(6.2.20)

Next, we take tangential derivative of the constitutive relation of Debye model defined at (6.2.8), and normal derivative of another one at (6.2.13) to obtain

\[
\gamma \frac{\partial^2 D_\tau}{\partial \tau \partial t} + \frac{\partial D_\tau}{\partial \tau} = \epsilon_0 \epsilon_\infty \gamma \frac{\partial^2 E_\tau}{\partial \tau \partial t} + \epsilon_0 \epsilon_s \frac{\partial E_\tau}{\partial \tau},
\]  

(6.2.21)

\[
\gamma \frac{\partial^2 D_n}{\partial n \partial t} + \frac{\partial D_n}{\partial n} = \epsilon_0 \gamma \frac{\partial}{\partial n} \left( \epsilon_\infty \frac{\partial E_n}{\partial t} \right) + \epsilon_0 \frac{\partial}{\partial n} (\epsilon_s E_n).
\]  

(6.2.22)

We now add Eqs. (6.2.21) and (6.2.22) together and simplify them by using the relation (6.2.20), and a condition that \( \epsilon_s \) and \( \epsilon_\infty \) are piecewise constant across the interface \( \Gamma \)

\[
0 = \gamma \epsilon_\infty \frac{\partial}{\partial t} \left( \frac{\partial E_\tau}{\partial \tau} + \frac{\partial E_n}{\partial n} \right) + \epsilon_s \left( \frac{\partial E_\tau}{\partial \tau} + \frac{\partial E_n}{\partial n} \right).
\]  

(6.2.23)

Let \( \Phi = \frac{\partial E_\tau}{\partial \tau} + \frac{\partial E_n}{\partial n} \) be a solution of ordinary differential equation (ODE) (6.2.23).
The first order jump condition of $E_n$ will be then evaluated as $[\partial E_n/\partial n] = [\Phi] - [\partial E_r/\partial \tau]$. Because $[\partial E_r/\partial \tau] = 0$ (due to (6.2.3)), we imply that

$$[\partial E_n/\partial n] = [\Phi]. \quad (6.2.24)$$

We note that with a given initial condition, solution $\Phi$ of ODE (6.2.23) is unique and explicitly computed at each time step. Specially, if the initial function is identical to zero, so is the solution of (6.2.23), which yields that $[\partial E_n/\partial n] = 0$. We again adopt the derivative operator (3.2.5) to evaluate $[\partial E_n/\partial n]$ in the Cartesian coordinate system

$$[\Phi] = \left[ \frac{\partial E_n}{\partial n} \right] = \cos^2 \theta \left[ \frac{\partial E_x}{\partial x} \right] + \cos \theta \sin \theta \left[ \frac{\partial E_y}{\partial x} \right] + \cos \theta \sin \theta \left[ \frac{\partial E_x}{\partial y} \right] + \sin^2 \theta \left[ \frac{\partial E_y}{\partial y} \right]. \quad (6.2.25)$$

The last linearly independent equation can be accomplished by contemplating term $[\partial E_n/\partial t]$. We again manipulate the constitutive relation of Debye material by taking tangential derivative of Eq. (6.2.13)

$$\gamma \frac{\partial^2 D_n}{\partial \tau \partial t} + \frac{\partial D_n}{\partial \tau} = \epsilon_0 \epsilon_\infty \frac{\partial^2 E_n}{\partial \tau \partial t} + \epsilon_0 \epsilon_s \frac{\partial E_n}{\partial \tau}. \quad (6.2.26)$$

To make an appearance of the jump term $[\partial E_n/\partial t]$ in Eq. (6.2.26), one can take jump operator to it, and recall the fact that $[\partial D_n/\partial \tau] = 0$

$$0 = \gamma \left[ \frac{\partial^2 D_n}{\partial \tau \partial t} \right] + \left[ \frac{\partial D_n}{\partial \tau} \right] = \epsilon_0 \epsilon_\infty \gamma \left[ \frac{\partial^2 E_n}{\partial \tau \partial t} \right] + \epsilon_0 \epsilon_s \left[ \frac{\partial E_n}{\partial \tau} \right]. \quad (6.2.27)$$

Now, let $\psi_{E_n}(t, x, y) = [\partial E_n/\partial \tau]$, and the same algebraic modification as of (6.2.14) is taken into account to get a new IADE

$$\gamma \epsilon^- \frac{\partial \psi_{E_n}}{\partial t} = -\epsilon^- \psi_{E_n} - \gamma \left( \epsilon^+ - \epsilon^- \right) \frac{\partial}{\partial t} \left( \frac{\partial E_n}{\partial \tau} \right)^+ - (\epsilon^+ - \epsilon^-) \left( \frac{\partial E_n}{\partial \tau} \right)^+, \quad (6.2.28)$$
in which

\[
\left( \frac{\partial E_n}{\partial \tau} \right)^+ = - \sin \theta \cos \theta \left( \frac{\partial E_x}{\partial x} \right)^+ - \sin^2 \theta \left( \frac{\partial E_y}{\partial x} \right)^+ + \cos^2 \theta \left( \frac{\partial E_x}{\partial y} \right)^+ + \cos \theta \sin \theta \left( \frac{\partial E_y}{\partial y} \right)^+.
\]  

(6.2.29)

When value of \( \psi_{E_n}(t, x, y) = [\partial E_n / \partial \tau] \) is specified, we can refer it to the jump conditions of the electric components in the Cartesian grid as follows

\[
\psi_{E_n} = \left[ \frac{\partial E_n}{\partial \tau} \right] = - \sin \theta \cos \theta \left[ \frac{\partial E_x}{\partial x} \right] - \sin^2 \theta \left[ \frac{\partial E_y}{\partial x} \right] + \cos^2 \theta \left[ \frac{\partial E_x}{\partial y} \right] + \cos \theta \sin \theta \left[ \frac{\partial E_y}{\partial y} \right].
\]  

(6.2.30)

By solving four linearly independent equations (6.2.17), (6.2.19), (6.2.25), and (6.2.30), we obtain the first order jump conditions for the electric components in the Cartesian coordinate system as

\[
\left[ \frac{\partial E_x}{\partial y} \right] = \left[ \frac{\partial E_y}{\partial x} \right] = (\cos^2 \theta - \sin^2 \theta) \psi_{E_n} + \cos \theta \sin \theta \psi_{E_n}. \tag{6.2.31}
\]

The jump conditions of the electric fields are now completely known by looking at relations specified at (6.2.16) and (6.2.31). To sum up, the interface conditions for our fields needed to model the TE\(_z\) mode are given as below

1. for \( H_z \):

\[
[H_z] = 0, \quad \left[ \frac{\partial H_z}{\partial x} \right] = - \cos \theta \frac{\partial \psi_{D_z}}{\partial t}, \quad \left[ \frac{\partial H_z}{\partial y} \right] = - \sin \theta \frac{\partial \psi_{D_z}}{\partial t}. \tag{6.2.32}
\]

2. for \( E_x \):

\[
[E_x] = \cos \theta \psi_{E_n}, \quad \left[ \frac{\partial E_x}{\partial y} \right] = (\cos^2 \theta - \sin^2 \theta) \psi_{E_n} + \cos \theta \sin \theta \psi_{E_n}. \tag{6.2.33}
\]
for $E_y$:

$$[E_y] = \sin \theta \psi_{E_n}, \quad \left[ \frac{\partial E_y}{\partial x} \right] = (\cos^2 \theta - \sin^2 \theta) \psi_{E_n r} + \cos \theta \sin \theta \psi_{E_n} .$$  \hspace{1cm} (6.2.34)

It is worth noticing that the jump conditions of our fields declared at (6.2.32), (6.2.33), and (6.2.34) are decoupled and only one-dimensionally dependent. This property also features a principal idea in the matched interface boundary (MIB) method [26, 34] which is the two-dimensional (2D) jump condition should be decomposed into 1D ones in each Cartesian line. Nevertheless, the variables $\psi_{D_r}, \psi_{E_n}, \psi_{E_n r},$ and $\psi_{E_n}$ are unknown, but could be found by numerically solving the aforementioned IADEs. Unlike the magnetic mode (TM) discussed in Chapters 4 and 5, the TE mode in this work produces discontinuous solutions even with magnetic permeability being constant. Indeed, based on the interface conditions (6.2.32), (6.2.33), and (6.2.34), $H_z$ will belong to $C^0$, $E_x$ and $E_y$ are discontinuous functions across the interface. Therefore, the need to use interface schemes like MIB method is indispensable if one desires to achieve high order accuracy for field solutions.

### 6.2.3 Time discretization scheme

In our previous MIBTD methods (see Chapters 4, 5), a modified Maxwell system to model TM mode is proposed to exploit $\partial E_z/\partial t$ instead of $D_z$. However, in this present work, a standard Maxwell system including Eqs. (6.1.1) to (6.1.5) is employed due to the need of the jump conditions of $D_z$. The leapfrog scheme is found to be effectively used when discretizing IADEs. For convenience to integrate the leapfrog scheme into our system, we adopt notations presented in Section 2.5.2. In this time-stepping algorithm, the time positions of our field components are placed in a leapfrog manner, see Fig. 6.1. More specifically, while magnetic component $H_z$ located at a discrete time $t_k$, the rest of all TE mode’s fields such as $E_x, E_y, D_x, \text{and } D_y$ are evaluated at $t_{k+\frac{1}{2}} = t_k + \frac{\Delta t}{2}$.

Under the leapfrog arrangement, to evaluate first order jump conditions of $H_z$ component
at a discrete time $t_{k+1}$, one should study IADE (6.2.10) at $t_{k+\frac{1}{2}}$ and at arbitrary point $(x_o, y_o)$ on the interface $\Gamma$. For short, we denote $u|_k$ as $u|_{k(x,y)}$

$$\gamma \left( \frac{\psi_{D_x}^{k+\frac{1}{2}}}{\Delta t} + \psi_{D_x}^{k+\frac{1}{2}} \right) = \epsilon_0 \gamma \left( \epsilon_+^{\infty} - \epsilon_-^{\infty} \right) \frac{\partial E^+_{\tau}}{\partial t}|_{k+\frac{1}{2}} + \epsilon_0 \left( \epsilon_+^s - \epsilon_-^s \right) E^+_{\tau}|_{k+\frac{1}{2}}, \quad (6.2.35)$$

By employing Yee’s expressions (see Section 2.5), Eq. (6.2.35) will be discretized in time as

$$\gamma \left( \frac{\psi_{D_x}^{k+1} - \psi_{D_x}^k}{\Delta t} \right) + \psi_{D_x}^{k+1} + \frac{\psi_{D_x}^k}{2} = \epsilon_0 \gamma \left( \epsilon_+^{\infty} - \epsilon_-^{\infty} \right) \frac{E^+_{\tau}|_{k+\frac{1}{2}} - E^+_{\tau}|_{k-\frac{1}{2}}}{\Delta t}$$

$$+ \epsilon_0 \left( \epsilon_+^s - \epsilon_-^s \right) E^+_{\tau}|_{k+\frac{1}{2}} + O(\Delta t). \quad (6.2.36)$$

Simplifying the above equation, one arrives at

$$\left( \frac{\gamma}{\Delta t} + \frac{1}{2} \right) \psi_{D_x}^{k+1} = \left( \frac{\gamma}{\Delta t} - \frac{1}{2} \right) \psi_{D_x}^k + \epsilon_0 \left( \epsilon_+^{\infty} - \epsilon_-^{\infty} \right) \frac{\epsilon_+^s - \epsilon_-^s}{\Delta t} E^+_{\tau}|_{k+\frac{1}{2}}$$

$$- \epsilon_0 \gamma \frac{\epsilon_+^{\infty} - \epsilon_-^{\infty}}{\Delta t} E^+_{\tau}|_{k-\frac{1}{2}} + O(\Delta t). \quad (6.2.37)$$

Since the time discretization above uses Euler-backward approximation on term $\frac{\partial E^+_{\tau}}{\partial t}|_{k+\frac{1}{2}}$, we
are only able to attain the first order in time $O(\Delta t)$ in our discretization (6.2.37). However, this drawback can be lessened by considering a small enough time step $\Delta t$, the spatial error will then dominate the temporal error. With $\psi_{D,r}|^{k+1}$ being valued in Eq. (6.2.37), the first order jump conditions of $H_z$ field (6.2.32) can be derived by adopting the following discretization

$$\frac{\psi_{D,r}}{\partial t}|^{k+1} = \frac{\psi_{D,r}|^{k+1} - \psi_{D,r}|^k}{\Delta t} + O(\Delta t). \tag{6.2.38}$$

We now estimate the zeroth order jump conditions of the electric fields at time step $k + \frac{3}{2}$ by taking into account IADE (6.2.14) at the discrete time $t_{k+1}$

$$\gamma\epsilon^- \frac{\partial \psi_{En}}{\partial t}|^{k+1} = -\epsilon_s^- \psi_{En}|^{k+1} - \gamma \left( \epsilon^+ - \epsilon^- \right) \frac{\partial E_n^+}{\partial t}|^{k+1} - \left( \epsilon_s^+ - \epsilon_s^- \right) E_n^+|^{k+1}. \tag{6.2.39}$$

The leapfrog algorithm gives us a following approximation form of (6.2.39) with a second order accuracy in time

$$\gamma\epsilon^- \frac{\psi_{En}|^{k+\frac{3}{2}} - \psi_{En}|^{k+\frac{1}{2}}}{\Delta t} = -\epsilon_s^- \frac{\psi_{En}|^{k+\frac{3}{2}} + \psi_{En}|^{k+\frac{1}{2}}}{2} - \gamma \left( \epsilon^+ - \epsilon^- \right) \frac{E_n^+|^{k+\frac{3}{2}} - E_n^+|^{k+\frac{1}{2}}}{\Delta t}$$

$$- \left( \epsilon_s^+ - \epsilon_s^- \right) \frac{E_n^+|^{k+\frac{3}{2}} + E_n^+|^{k+\frac{1}{2}}}{2} + O(\Delta t^2) \tag{6.2.40}$$

$$\left( \frac{\gamma\epsilon^-}{\Delta t} + \frac{\epsilon_s^-}{2} \right) \psi_{En}|^{k+\frac{3}{2}} = \left( \frac{\gamma\epsilon^-}{\Delta t} - \frac{\epsilon_s^-}{2} \right) \psi_{En}|^{k+\frac{1}{2}} - \left\{ \frac{\gamma \left( \epsilon^+ - \epsilon^- \right)}{\Delta t} \frac{\epsilon_s^+ - \epsilon_s^-}{2} \right\} E_n^+|^{k+\frac{1}{2}}$$

$$+ \left\{ \frac{\gamma \left( \epsilon^+ - \epsilon^- \right)}{\Delta t} - \frac{\epsilon_s^+ - \epsilon_s^-}{2} \right\} E_n^+|^{k+\frac{1}{2}} + O(\Delta t^2). \tag{6.2.41}$$

By carrying out the same approach as of $\psi_{En}$’s discretization on IADE (6.2.28), the value of $\psi_{E_{nr}}$ is numerically evaluated as follows

$$\left( \frac{\gamma\epsilon^-}{\Delta t} + \frac{\epsilon_s^-}{2} \right) \psi_{E_{nr}}|^{k+\frac{3}{2}} = \left( \frac{\gamma\epsilon^-}{\Delta t} - \frac{\epsilon_s^-}{2} \right) \psi_{E_{nr}}|^{k+\frac{1}{2}} - \left\{ \frac{\gamma \left( \epsilon^+ - \epsilon^- \right)}{\Delta t} \frac{\epsilon_s^+ - \epsilon_s^-}{2} \right\} \frac{\partial E_n^+}{\partial \tau}|^{k+\frac{3}{2}}$$

$$+ \left\{ \frac{\gamma \left( \epsilon^+ - \epsilon^- \right)}{\Delta t} - \frac{\epsilon_s^+ - \epsilon_s^-}{2} \right\} \frac{\partial E_n^+}{\partial \tau}|^{k+\frac{1}{2}} + O(\Delta t^2). \tag{6.2.42}$$
Unlike the other interface terms $\psi_{E_n}$ and $\psi_{E_{n+\tau}}$, unknown value $\psi_{E_{n+\tau}}$ is determined by using the identity (6.2.24) the analytical solution of ODE (6.2.23) rather than employing the time-stepping scheme on IADE. Furthermore, Maxwell’s equations (6.1.1)–(6.1.5) will be discretized in time via the leapfrog scheme as follows

\begin{align*}
H_z^{k+1} &= H_z^k - \frac{\Delta t}{\mu} \left( \frac{\partial E_y^{k+\frac{1}{2}}}{\partial y} - \frac{\partial E_y^{k+\frac{1}{2}}}{\partial x} \right) + O(\Delta t^3) \quad (6.2.43) \\
D_x^{k+\frac{3}{2}} &= D_x^{k+\frac{1}{2}} + \Delta t \frac{\partial H_z^{k+1}}{\partial y} + O(\Delta t^3) \quad (6.2.44) \\
D_y^{k+\frac{3}{2}} &= D_y^{k+\frac{1}{2}} - \Delta t \frac{\partial H_z^{k+1}}{\partial x} + O(\Delta t^3) \quad (6.2.45)
\end{align*}

\begin{align*}
\left( \frac{\epsilon_0 \epsilon_{\infty}}{\Delta t} + \frac{\epsilon_0 \epsilon_s}{2} \right) E_x^{k+\frac{3}{2}} &= \left( \frac{\epsilon_0 \epsilon_{\infty}}{\Delta t} - \frac{\epsilon_0 \epsilon_s}{2} \right) E_x^{k+\frac{1}{2}} + \left( \frac{\gamma}{\Delta t} + \frac{1}{2} \right) D_x^{k+\frac{3}{2}} \\
&\quad + \left( -\frac{\gamma}{\Delta t} + \frac{1}{2} \right) D_x^{k+\frac{1}{2}} + O(\Delta t^2) \quad (6.2.46) \\
\left( \frac{\epsilon_0 \epsilon_{\infty}}{\Delta t} + \frac{\epsilon_0 \epsilon_s}{2} \right) E_y^{k+\frac{3}{2}} &= \left( \frac{\epsilon_0 \epsilon_{\infty}}{\Delta t} - \frac{\epsilon_0 \epsilon_s}{2} \right) E_y^{k+\frac{1}{2}} + \left( \frac{\gamma}{\Delta t} + \frac{1}{2} \right) D_x^{k+\frac{3}{2}} \\
&\quad + \left( -\frac{\gamma}{\Delta t} + \frac{1}{2} \right) D_y^{k+\frac{1}{2}} + O(\Delta t^2) \quad (6.2.47)
\end{align*}

Note that all discretizations in time-domain are fully explicit because the values at the current discrete time are computed by the previous ones; therefore, a deal with solving simultaneous equations and matrix inversion is avoided.

In our algorithm, the staggered grid is employed for our finite-difference method, see Fig. 2.1. This kind of lattice is considered due to the purpose of preserving the divergence-free condition and stability reinforcement. This subsection features an extrapolation form of the node on the interface and the matched interface and boundary (MIB) method for both small and large interface curvature.
6.2.4 One-sided extrapolation scheme

In our algorithm, the staggered grid is employed for our finite-difference method, see Fig. 2.1. This kind of lattice is considered due to the purpose of preserving the divergence-free condition and stability reinforcement. Unlike the formulations of IADEs for TM mode reported in the previous Chapters 4 and 5, the expressions of IADEs for TE mode in this work involve interpolations of the different fields having staggered locations. That highlight gives rise to some difficulties in dealing with complex interfaces. For an illustration of this matter, we study the extrapolation form of the one-sided term \( \frac{\partial E_+}{\partial \tau} \bigg|_{k+\frac{1}{2}} \) appearing in (6.2.28).

It is noted that the one-sided function is always evaluated at a point on the interface. By considering a random point \((x_o, y_o)\) on the interface \(\Gamma\), see Fig. 6.2, \( \frac{\partial E_+}{\partial \tau} \bigg|_{k+\frac{1}{2}} \) then can be calculated based on the expression (6.2.29) at that point as

\[
\frac{\partial E_+^x}{\partial \tau} \bigg|_{(x_o, y_o)}^{k+\frac{1}{2}} = -\sin \theta \cos \theta \frac{\partial E_+^x}{\partial x} \bigg|_{(x_o, y_o)}^{k+\frac{1}{2}} - \sin^2 \theta \frac{\partial E_+^y}{\partial x} \bigg|_{(x_o, y_o)}^{k+\frac{1}{2}} + \cos^2 \theta \frac{\partial E_+^x}{\partial y} \bigg|_{(x_o, y_o)}^{k+\frac{1}{2}} \\
+ \cos \theta \sin \theta \frac{\partial E_+^y}{\partial y} \bigg|_{(x_o, y_o)}^{k+\frac{1}{2}}.
\]

(6.2.48)

We will classify the interface point \((x_o, y_o)\) as \(x\)-point if it is the intersection between the interface \(\Gamma\) and \(x\)-line, and as \(y\)-point if it is the intersection between the interface \(\Gamma\) and \(y\)-line. Without the loss of general, we assume \((x_o, y_o)\) to be \(x\)-point with \(x_{i-1} < x_o < x_{i-\frac{1}{2}}\), \(y_o = y_j\), \((x_{i-1}, y_j)\) and \((x_o, y_{j-\frac{1}{2}})\) \(\in \Omega^-\), \((x_{i-\frac{1}{2}}, y_j)\) and \((x_o, y_{j+\frac{1}{2}})\) \(\in \Omega^+\), see Fig. 6.2. Based on the local shape of the interface nearby the interface node \((x_o, y_o)\), we design two different approaches for the one-sided extrapolation method.

**Horizontal approach:** In this approach, the function values in our IADEs are first extrapolated along the horizontal direction, i.e. \(x\)-line. For instance, to approximate the value of \(E_y^+\) and its derivative at the interface point \((x_o, y_o)\), we will deploy three function
values defined at grid nodes \((i - \frac{1}{2}, j), (i + \frac{1}{2}, j)\) and \((i + \frac{3}{2}, j)\)

\[
E_y^+ |_{(x_o, y_o)} = w_{0,1}^+ E_y|_{i-\frac{1}{2},j} + w_{0,2}^+ E_y|_{i+\frac{1}{2},j} + w_{0,3}^+ E_y|_{i+\frac{3}{2},j} + O(\Delta x^2), \tag{6.2.49}
\]

\[
\frac{\partial E_y^+}{\partial x} |_{(x_o, y_o)} = w_{1,1}^+ E_y|_{i-\frac{1}{2},j} + w_{1,2}^+ E_y|_{i+\frac{1}{2},j} + w_{1,3}^+ E_y|_{i+\frac{3}{2},j} + O(\Delta x^2). \tag{6.2.50}
\]

where \(\{w_{l,k}^+ \mid l = 0,1; k = 1,2,3\}\) are one-sided difference weights used in the positive subdomain \(\Omega^+\). In addition, \(l = 0\) is for the interpolation and \(l = 1\) is for the first derivative approximation, and \(k\) is for the grid index. Note that, we dismiss the superscript regarding time-step in the above discretizations for short.

To estimate one-sided term \(\frac{\partial E_y^+}{\partial y}\) at \((x_o, y_o)\), we first interpolate it along the horizontal by
using the same sets of grid points employed in approximating \( E_y \)

\[
\left. \frac{\partial E_y^+}{\partial y} \right|_{(x_o, y_o)} = w_{0,1}^+ \left. \frac{\partial E_y^+}{\partial y} \right|_{i-\frac{1}{2},j} + w_{0,2}^+ \left. \frac{\partial E_y^+}{\partial y} \right|_{i+\frac{1}{2},j} + w_{0,3}^+ \left. \frac{\partial E_y^+}{\partial y} \right|_{i+\frac{3}{2},j} + O(\Delta x^2), \quad (6.2.51)
\]

then we use add two more grid nodes (pink circles in Fig. 6.2) along each vertical line to derive the first derivative of \( E_y \) at three previous nodes, see Fig. 6.2. Specifically, the approximation form of \( \left. \frac{\partial E_y^+}{\partial y} \right|_{i-\frac{1}{2},j} \) will be interpolated as follows

\[
\left. \frac{\partial E_y^+}{\partial y} \right|_{i-\frac{1}{2},j} = p_{1,1}^+ E_y|_{i-\frac{1}{2},j} + p_{1,1}^+ E_y|_{i-\frac{1}{2},j+1} + p_{1,3}^+ E_y|_{i-\frac{1}{2},j+2} + O(\Delta y^2), \quad (6.2.52)
\]

here \( p_{l,k}^+ \) are one-sided difference weights. Note that the two remaining terms \( \left. \frac{\partial E_y^+}{\partial y} \right|_{i+\frac{1}{2},j} \) and \( \left. \frac{\partial E_y^+}{\partial y} \right|_{i+\frac{3}{2},j} \) in (6.2.51) will be evaluated in the same manner as of (6.2.52).

To interpolate the value of \( E_x \) and its derivatives at the interface point \((x_o, y_o)\), we also firstly utilize three auxiliary points of \( E_x \) at \((i, j)\), \((i + 1, j)\) and \((i + 2, j)\) to obtain the following estimations

\[
E_x^+|_{(x_o, y_o)} = \tilde{w}_{0,1}^+ E_x|_{i,j} + \tilde{w}_{0,2}^+ E_x|_{i+1,j} + \tilde{w}_{0,3}^+ E_x|_{i+2,j} + O(\Delta x^2), \quad (6.2.53)
\]

\[
\left. \frac{\partial E_x^+}{\partial x} \right|_{(x_o, y_o)} = \tilde{w}_{1,1}^+ E_x|_{i,j} + \tilde{w}_{1,2}^+ E_x|_{i+\frac{1}{2},j} + \tilde{w}_{1,3}^+ E_x|_{i+\frac{3}{2},j} + O(\Delta x^2), \quad (6.2.54)
\]

\[
\left. \frac{\partial E_x^+}{\partial y} \right|_{(x_o, y_o)} = \tilde{w}_{0,1}^+ \left. \frac{\partial E_x^+}{\partial y} \right|_{i,j} + \tilde{w}_{0,2}^+ \left. \frac{\partial E_x^+}{\partial y} \right|_{i+\frac{1}{2},j} + \tilde{w}_{0,3}^+ \left. \frac{\partial E_x^+}{\partial y} \right|_{i+\frac{3}{2},j} + O(\Delta x^2). \quad (6.2.55)
\]

where \( \tilde{w}_{l,k}^+ \) are one-sided finite difference weights. To be aware of that all the values on the right hand sides of (6.2.53), (6.2.54), and (6.2.55) are determined on the auxiliary nodes of \( E_x \) fields. Therefore, they have to be further implemented by making the use of three grid nodes along the vertical line for each approximation (see the orange squares in Fig. 6.2. For example, by referring to Fig. 6.2), the extrapolation of \( E_x|_{i,j} \) along the \( y \)-line will involve three grid points \((i, j - \frac{1}{2}), (i, j + \frac{1}{2})\) and \((i, j + \frac{3}{2})\). Keep in mind that we always have to
use at least three function values for each interpolation so that the second order accuracy in space could be maintained.

**Vertical approach:** This algorithm will firstly interpolate the function values by using nodes vertically aligned, the auxiliary values will be then estimated along the desired directions if necessary. If one wants to approximate the $E_y$ and its derivatives at the interface point $(x_o, y_o)$, three auxiliary nodes defined at locations $(x_o, y_{j+1}), (x_o, y_{j+2})$ and $(x_o, y_{j+3})$ (marked by open circles in Fig. 6.3) are taken into consideration. Since these values are evaluated on the auxiliary positions, they have to be represented by grid nodes for $E_y$ along the horizontal line. For example, the value of $E_y$ at $(x_o, y_{j+1})$ could be interpolated by using three points $(i - \frac{1}{2}, j + 1), (i + \frac{1}{2}, j + 1)$ and $(i + \frac{3}{2}, j + 1)$. We omit the details of the
Figure 6.4: Illustration of the possible cases for one-sided scheme. Open triangle: interface node; Filled circles: grid nodes for $E_y$; Filled squares: grid nodes for $E_x$. Left: vertical approach is applicable; Middle: horizontal approach is applicable; Right: both vertical and horizontal approaches (in the positive domain) are not applicable.

discretization form for this approach here because they are the same as the approximation forms already discussed in the horizontal approach. The extrapolation process for valuing $E_x$ and its derivatives will be conducted in the same manner as of $E_y$. The details of the node arrangement for the discretizations can be seen in Fig. 6.3.

Note that in both horizontal and vertical approaches, there are at least three grid/auxiliary nodes to be involved so that the second order accuracy is achieved in all the dissertations. Keep in mind that, the approaches from the negative direction could be conducted in the same manner. However, when the interface shape is very complex, in some cases, either one of the horizontal and vertical approaches can be applicable. Refer to Fig. 6.4, in the left figure, only the vertical approach from either positive or negative direction is able to use to attain the second order accuracy. In the middle figure of Fig. 6.4, only the horizontal approaches are appropriate. As can be seen in the right figure of Fig. 6.4, since there are not enough grid points for both positive-direction horizontal and vertical approaches, only negative-direction approaches can guarantee us a high order accuracy. It could be argued that the obstacles demonstrated in Fig. 6.4 may be avoided if a finer mesh is taken into account. But in practice, one still wants to employ the larger mesh sizes to verify the numerical convergences and to save the computational time. By considering the horizontal
and vertical algorithms, one can have at least one possible way to discretize IADEs even the shape of interface is not regular and the mesh is not dense enough.

6.2.5 A summary for MIB method combined with leapfrog scheme

To restore the second-order accuracy for the waves’ solution across the interface, we still employ the MIB schemes reported in Sections 4.2.4.1 and 4.2.4.2 to handle the small curvature and large curvature interfaces, respectively.

In this section, we summarize the stages of the MIB time-domain (MIBTD), i.e. the MIB algorithm based on the leapfrog scheme. Let assume that

• at $t_{k-\frac{1}{2}}$: $E_x$ and $E_y$ are given.

• at $t_k$: $H_z$ and $\psi_{D_r}$ are given.

• at $t_{k+\frac{1}{2}}$: $E_x$, $E_y$, $D_x$, $D_y$, $\psi_{E_n}$ and $\psi_{E_nr}$ are given.

The values for the next time step will be then determined by the following process

**Step 1.** use (6.2.43) to update values of $H_z$ at $t_{k+1}$.

**Step 2.** use (6.2.37) to update $\psi_{D_r}$ at $t_{k+1}$. First order jump conditions of $H_z$ will be then available at $t_{k+1}$ thanks to (6.2.32) and (6.2.38).

**Step 3.** enforce (6.2.32) to determine fictitious vales of $H_z$ at $t_{k+1}$.

**Step 4.** use (6.2.44) and (6.2.45) to evaluate $D_x$ and $D_y$ at $t_{k+\frac{3}{2}}$, respectively.

**Step 5.** use (6.2.46) and (6.2.47) to evaluate $E_x$ and $E_y$ at $t_{k+\frac{3}{2}}$, respectively.

**Step 6.** use (6.2.41) and (6.2.42) to update $\psi_{E_n}$ and $\psi_{E_n r}$ at $t_{k+\frac{3}{2}}$, respectively; use (6.2.24) to update $\psi_{E_{nn}}$ at $t_{k+\frac{3}{2}}$. Jump conditions of $E_x$ and $E_y$ will be then evaluated at $t_{k+\frac{3}{2}}$ thanks to (6.2.33) and (6.2.34).

**Step 7.** enforce (6.2.33) to determine fictitious values of $E_x$ at $t_{k+\frac{3}{2}}$; enforce (6.2.34) to determine fictitious values of $E_y$ at $t_{k+\frac{3}{2}}$. 

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6.3 Numerical Experiments

In this section, numerous numerical results are provided to validate our proposed MIB method combined with the leapfrog scheme. Different interface shapes with constant and non-constant curvatures, namely, circular, n-leaf rose, and bean interfaces in a square domain $[0 \text{ mm}, 30 \text{ mm}]^2$ are investigated in our numerical tests. Similar to the TM case reported in Chapter 4, the medium inside the interface is assigned to be water with Debye parameters: $\epsilon_s = 81$, $\epsilon_\infty = 1.8$, and $\gamma = 9.4 \text{ ps}$. A uniform mesh for the $H_z$ solution is carried out in all our simulations, in which number of grid points in both $x$ and $y$ are equal, i.e. $N_x = N_y$. For convenience, we denote $N = N_x = N_y$. The grid points for $E_x$, $E_y$, $D_x$, and $D_y$ components will be then formed in a staggered manner. In every our test, an incident pulse of the form $H_z(x, y, t) = \exp(- (x + 15 - c_0 t)^2/(2 \alpha^2))$ excited at an initial time $t = 0 \text{ ps}$ is imposed as a boundary condition at the left boundary $x = 0 \text{ mm}$, at the top boundary $y = 30 \text{ mm}$ and at the bottom boundary $y = 0 \text{ mm}$. Here $c_0$ is the speed of light in air, and $\alpha = 2.5 \text{ mm}$. Also, for simplicity, the PEC condition (see Section 2.6) is enforced on the right boundary $x = 30 \text{ mm}$. Our simulations will stop before the propagating waves hit the right boundary, and the reflected waves touch the bottom and top boundaries. Therefore, the stopping time $T$ is chosen to be $110 \text{ ps}$; also all our following experiments will be conducted at that time. With $N_t$ indicating number of time steps, the time increment is defined by $\Delta t = N_t/T$. Both relative $L_\infty$ and $L_2$ error measurements are utilized in our numerical tests and defined as follows

$$L_\infty = \frac{\max |u - u_h|}{\max |u|}, \quad L_2 = \sqrt{\frac{\sum |u - u_h|^2}{\sum |u|^2}}, \quad (6.3.1)$$

where $u$ and $u_h$ are, respectively, the reference solution and numerical solution.
6.3.1 Example 1: Circular dispersive interface

We first consider the circular interface $\Gamma$ defined by

$$\Gamma : \sqrt{(x - 6\pi)^2 + (y - 15)^2} = \frac{100}{23},$$

(6.3.2)

where the unit is in millimeters. For a comparison, we also employ the FDTD based on the leapfrog scheme to discretize Maxwell system including Eqs. (6.1.1)–(6.1.5). Note that the FDTD basically shares the same boundary conditions, spatial discretizations and temporal discretizations with the MIBTD method, except for the interface treatment. We firstly investigate the stability of the proposed MIBTD and FDTD algorithms. By referring to Section 2.5.5, the Courant-Friedrichs-Lewy (CFL) stability condition for solving Maxwell's equations in 2D is specified as

$$\Delta t \leq C \frac{\Delta x}{c_0 \sqrt{2}}.$$

(6.3.3)

It is obvious to see that the CFL constant $C$ is determined by the spatial and temporal increments. Here we are interested in numerically evaluating the value of $C$ by studying a critical $N_t$ value for a given number of grid points $N$. The critical $N_t$ value, denoted by $N_t^*$, is defined in a sense the same as in Chapter 4, i.e only $N_t$ values smaller than $N_t^*$ will render our computational solution unstable. Table 6.1 reports values of $N_t^*$ and values of CFL constant $C$ based on different mesh sizes. In particular, while spatial increment $\Delta x$ approaches 0, the CFL number $C$ of the FDTD scheme goes to 1. In fact, $C = 1$ is a theoretical CFL number of the FDTD method for solving non-dispersive interface problems (Section 2.5.5).

It can be seen from Table 6.1 that the CFL numbers of the MIBTD algorithm are very close to the corresponding values of its counterpart when considering dense meshes. Therefore, it seems that in comparison to the classical scheme, our proposed method does not significantly reduce the stability even many interface treatments are carried out in this algorithm.

In our next study, the numerical accuracy and convergence are taken into consideration. It is just a reminder that we investigate the numerical results of both MIBTD and FDTD.
Table 6.1: Critical CFL number $C$ for the circular interface problem in TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$\text{FDTD}$</th>
<th>MIBTD</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$N_t^*$</td>
<td>$C$</td>
</tr>
<tr>
<td>101</td>
<td>155</td>
<td>1.0029</td>
</tr>
<tr>
<td>161</td>
<td>248</td>
<td>1.0029</td>
</tr>
<tr>
<td>201</td>
<td>311</td>
<td>0.9997</td>
</tr>
<tr>
<td>321</td>
<td>497</td>
<td>1.0009</td>
</tr>
<tr>
<td>401</td>
<td>622</td>
<td>0.9997</td>
</tr>
</tbody>
</table>

Table 6.2: Numerical convergence test of the circular dispersive interface problem in the TE mode in the relative $L_\infty$ and $L_2$ norms.

<table>
<thead>
<tr>
<th>$N$</th>
<th>$L_\infty$ norm</th>
<th>$L_2$ norm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD</td>
<td>MIBTD</td>
</tr>
<tr>
<td></td>
<td>Error Order</td>
<td>Error Order</td>
</tr>
<tr>
<td>101</td>
<td>2.12E-01 0.34</td>
<td>3.14E-02 1.75</td>
</tr>
<tr>
<td>161</td>
<td>1.81E-01 0.95</td>
<td>9.70E-03 2.09</td>
</tr>
<tr>
<td>201</td>
<td>1.46E-01 1.00</td>
<td>6.10E-03 2.09</td>
</tr>
<tr>
<td>321</td>
<td>9.16E-02 1.00</td>
<td>2.30E-03 2.08</td>
</tr>
<tr>
<td>401</td>
<td>7.40E-02 0.96</td>
<td>1.50E-03 1.92</td>
</tr>
</tbody>
</table>

Figure 6.5: Numerical convergence tests for the circular dispersive interface problem in TE mode. Here, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.

methods at the stopping time $T = 110$ ps which is short enough to not allow the scattered waves hit the boundaries of the computational domain. To examine the rate of convergence, we employ the odd number grid points $N$ since there are no analytical solutions available for the dispersive interface problems. Therefore, to benchmark our scheme, a reference solution
Figure 6.6: The MIBTD solution with $N = 321$ at $t = 110$ ps for the circular dispersive interface problem in TE mode. (a) Contour plot of $H_z$. (b) $E_z(x, 15)$. (c) Contour plot of $E_y$. (d) $H_y(x, 17.81)$. (e) Contour plot of $E_x$. (f) $H_x(16.12, y)$. 

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is generated by the MIBTD algorithm at a dense mesh $N = 1601$ and a sufficiently small $\Delta t$. Due to the use of the numerically analytical solution, only special refined meshes are considered. Specifically, the tested mesh size $N$ must satisfy a condition that $N - 1$ is a divisor of 1601. To compute the error measurements for a numerical solution generated at a grid size $N$, we have to take into account the reference solution at a rate $1600/(N - 1)$, i.e. keeping one reference value in each $1600/(N - 1)$ values. The numerical solution will be then compared with that downsize reference one to attain the numerical errors. Thus, different mesh sizes $N = 101, 161, 201, 321$ and 401 are employed in the present study; and to ensure the stability, the CFL number $C = 0.6$ is used in both methods. Note that only error results for $H_z$ component are reported in all our tests. The convergence analysis for the rest of components are not applicable because their grid nodes are staggered to the $H_z$ nodes. Table 6.2 reports numerical errors and numerical orders in both $L_\infty$ and $L_2$ norms. It can be seen that our proposed method successfully achieved a second order convergence while the FDTD scheme fails to restore that desired accuracy. For illustration purpose, we depict both $L_\infty$ and $L_2$ errors of the tested schemes in Fig. 6.5. A linear least square fitting [34] is used to identify the overall numerical order of the algorithms. It can be read from Fig. 6.5 that the $L_\infty$ and $L_2$ errors of our MIBTD method are $s = 1.98$ and $s = 1.98$, respectively. As expected, the FDTD scheme without the proper interface treatment only attains numerical orders $s = 0.79$ in $L_\infty$ error norm, and $s = 0.91$ in $L_2$. These results indicate that our proposed method is superior to the classical one. Moreover, the contour and slice plots of the MIBTD solutions at grid node $N = 321$ are shown in Fig. 6.6. The slice plots clearly reveal that while $H_z$ solution is $C^0$, $E_y$ and $E_x$ solutions are only discontinuous across the interface.

The last test for this case concerns the computational speeds of MIBTD and FDTD methods. Table 6.3 reports the CPU time in seconds for both those algorithms. All computations here are conducted on an SGI Xeon E5-4640 CPU core operating at 2.4 GHz and 8 GB of memory. Similar to the accuracy test, CFL constant $C$ is assigned to be $C = 0.6$. 

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Table 6.3: CPU time in seconds of the FDTD method ($T_F$) and the MIBTD method ($T_M$) for the circular interface problem in TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>CPU time of FDTD ($T_F$)</th>
<th>CPU time of MIBTD ($T_M$)</th>
<th>$T_M/T_F$</th>
</tr>
</thead>
<tbody>
<tr>
<td>101</td>
<td>0.22</td>
<td>0.26</td>
<td>1.18</td>
</tr>
<tr>
<td>161</td>
<td>0.51</td>
<td>0.68</td>
<td>1.33</td>
</tr>
<tr>
<td>201</td>
<td>0.81</td>
<td>1.16</td>
<td>1.43</td>
</tr>
<tr>
<td>321</td>
<td>2.62</td>
<td>5.13</td>
<td>1.96</td>
</tr>
<tr>
<td>401</td>
<td>5.00</td>
<td>10.69</td>
<td>2.14</td>
</tr>
</tbody>
</table>

Table 6.3 reads that in every mesh refinement, the MIBTD method always consumes more CPU time than the FDTD method. When $N$ is large, the approximate ratio between the speed of our proposed method over that of the FDTD scheme is 2.14. That is reasonable since the MIBTD algorithm involves in solving IADEs and generating the fictitious values for the field components. However, when a certain high precision is interested, the MIBTD is indeed more cost-effective. For example, if one wants to achieve an accuracy of 7.40E-02 in $L_{\infty}$ norm, the FDTD method has to be conducted at $N = 401$. By referring to Table 6.3, that method will cost the amount of the CPU time as much as 5.00 seconds. However, our proposed method only needs to consider a coarse grid $N = 101$ to gain that precision. As a result, the computational time used by it is as low as $N = 0.26$ seconds. Therefore, the MIBTD method is clearly faster and more robust than its counterpart.

6.3.2 Example 2: $N$-leaf rose dispersive interface

We next examine more complex interfaces to illustrate the robustness of the MIBTD method. A family of interfaces named n-leaf rose is defined by the polar angle $\theta$ as in Section 4.3.2.3

$$\Gamma : \sqrt{(x-6\pi)^2 + (y-15)^2} = \frac{100}{23} + b \sin(m\theta), \quad \theta \in [0, 2\pi]. \quad (6.3.4)$$

The unit of this interface equation as well as $b$ is in millimeters. Four different interface shapes with parameters $(m, b) = (2, 5/2), (3, 5/4), (4, 10/9)$ and $(5, 1)$ are regarded as 2-leaf rose,
3–leaf rose, 4–leaf rose, and 5–leaf rose, respectively.

Table 6.4: Numerical convergence tests of the n–leaf rose dispersive interfaces in the $L_{\infty}$ norm in TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>2–leaf rose ($m = 2$, $b = 5/2$)</th>
<th>3–leaf rose ($m = 3$, $b = 5/4$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD Error, Order</td>
<td>MIBTD Error, Order</td>
</tr>
<tr>
<td>101</td>
<td>1.52E-1, 2.03E-2</td>
<td>2.12E-1, 2.82E-2</td>
</tr>
<tr>
<td>161</td>
<td>1.22E-1, 0.48</td>
<td>0.95</td>
</tr>
<tr>
<td>201</td>
<td>5.93E-2, 1.40E-3</td>
<td>1.08E-1, 7.29E-2</td>
</tr>
<tr>
<td>321</td>
<td>4.69E-2, 1.00E-3</td>
<td>0.95</td>
</tr>
</tbody>
</table>

Table 6.5: Numerical convergence tests of the n–leaf rose dispersive interfaces in the $L_2$ norm in TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>2–leaf rose ($m = 2$, $b = 5/2$)</th>
<th>3–leaf rose ($m = 3$, $b = 5/4$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD Error, Order</td>
<td>MIBTD Error, Order</td>
</tr>
<tr>
<td>101</td>
<td>1.78E-1, 3.57E-2</td>
<td>1.94E-1, 9.23E-2</td>
</tr>
<tr>
<td>161</td>
<td>1.25E-1, 0.75</td>
<td>0.75</td>
</tr>
<tr>
<td>201</td>
<td>1.09E-1, 0.65</td>
<td>1.23</td>
</tr>
<tr>
<td>321</td>
<td>6.98E-2, 0.94</td>
<td>0.52</td>
</tr>
<tr>
<td>401</td>
<td>6.30E-2, 0.46</td>
<td>0.37</td>
</tr>
</tbody>
</table>

We here only investigate the accuracy of the MIBTD method for these complex interfaces.
Since the stability and CPU time for this case is almost the same as the circular interface case, they will be omitted in this example to save space. Again, the CFL constant $C$ is chosen as $C = 0.6$ in all our tests; and a reference solution generated by the MIBTD algorithm at grid size $N = 1601$ and with a sufficiently small $\Delta t$. $L_\infty$ and $L_2$ errors and numerical orders for four different interface shapes, respectively, are reported in Table 6.4 and Table 6.5. By studying those data, we can apprehend that the MIBTD method always maintain the second-order accuracy even with highly complicated interfaces. As predicted, the regular FDTD scheme fails to restore the designed order due to the appearance of the jumps of the field solutions along the interface. Furthermore, the numerical errors in all the tests are depicted
in Fig. 6.7. Similar to the circular interface case, the least-square fitting tool is employed to detect the overall convergence orders of the tested methods. Thus, the numerical order $s_{L_\infty}$ for $L_\infty$ error and $s_{L_2}$ for $L_2$ error for the MIBTD method is found to be $s_{L_\infty} = 2.14$, $s_{L_2} = 1.91$ for 2–leaf rose case, $s_{L_\infty} = 2.21$, $s_{L_2} = 1.91$ for 3–leaf rose case, $s_{L_\infty} = 2.15$, $s_{L_2} = 2.29$ for 4–leaf rose case, and $s_{L_\infty} = 2.44$, $s_{L_2} = 2.47$ for 5–leaf rose case. It can be seen clearly in Fig. 6.7 that the FDTD method generally only attain first order in all cases. In particular, its numerical is found to be $s_{L_\infty} = 0.87$, $s_{L_2} = 0.72$ for 2–leaf rose case, $s_{L_\infty} = 0.93$, $s_{L_2} = 0.93$ for 3–leaf rose case, $s_{L_\infty} = 0.77$, $s_{L_2} = 0.94$ for 4–leaf rose case, and $s_{L_\infty} = 0.83$, $s_{L_2} = 0.85$ for 5–leaf rose case. It is clear to see in Figs 6.8, 6.9, 6.10, and 6.11 that $H_z$ is $C^0$ across the interface, and $E_x$ and $E_y$ are the discontinuous solutions.

6.3.3 Example 3: Bean-shaped dispersive interface

To demonstrate the performance of the MIBTD method, we consider another complex interface family, namely bean-shaped interface. This kind of interfaces is defined in the polar coordinate as follows

$$
\Gamma : \sqrt{(x - 6\pi)^2 + (y - 15)^2} = -\frac{150}{23} (\sin^n(\theta) + \cos^m(\theta)), \quad \theta \in [0, 2\pi].
$$

(6.3.5)

Note that the unit of the interface equations is in millimeters. Here the parameters $n$ and $m$ determine how much the bean-shaped curve is compressed in from a regular circle; in particular, $n$ is for the vertical-direction press and $m$ is for the horizontal-direction press. Two different bean-shaped interfaces with parameters $(n, m) = (3, 3)$ and $(1, 15)$ are regarded as Case 3(a) and Case 3(b). It is noticed that the latter interface shape has a larger curvature than that of the first one. Therefore, the use of the MIB treatment designed for the large curvature interface for the case 3(b) is indispensable. Since the impact of the Bean-shaped interface on the stability condition and the execution time of the MIBTD method is negligible, those tests will not be presented here.
Figure 6.8: The MIBTD solution with $N = 321$ at $t = 110$ ps for the 2–leaf rose interface with parameters $(b, m) = (2, 5/2)$ in TE mode. (a) Contour plot of $H_z$. (b) $H_z(x, 11.25)$. (c) Contour plot of $E_y$. (d) $E_y(x, 9.84)$. (e) Contour plot of $E_x$. (f) $E_x(19.69, y)$. 
Figure 6.9: The MIBTD solution with $N = 321$ at $t = 110$ ps for the 3–leaf rose interface with parameters $(b, m) = (3, 5/4)$ in TE mode. (a) Contour plot of $H_z$. (b) $H_z(15.74, y)$. (c) Contour plot of $E_y$. (d) $E_y(x, 18.75)$. (e) Contour plot of $E_x$. (f) $E_x(15.56, y)$.
Figure 6.10: The MIBTD solution with $N = 321$ at $t = 110$ ps for the 4–leaf rose interface with parameters $(b, m) = (4, 10/9)$ in TE mode. (a) Contour plot of $H_z$. (b) $H_z(x, 18.28)$. (c) Contour plot of $E_y$. (d) $E_y(x, 10.31)$. (e) Contour plot of $E_x$. (f) $E_x(14.53, y)$. 
Figure 6.11: The MIBTD solution with $N = 321$ at $t = 110$ ps for the 5–leaf rose interface with parameters $(b, m) = (5, 1)$ in TE mode. (a) Contour plot of $H_z$. (b) $H_z(15.38, y)$. (c) Contour plot of $E_y$. (d) $E_y(x, 10.97)$. (e) Contour plot of $E_x$. (f) $E_x(15.38, y)$. 

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Table 6.6: Numerical convergence tests of the bean-shaped dispersive interfaces in the $L_\infty$ and $L_2$ norm in TE mode.

<table>
<thead>
<tr>
<th>$N$</th>
<th>Case 3(a): $n = 3$, $m = 3$ ($L_\infty$)</th>
<th>Case 3(a): $n = 3$, $m = 3$ ($L_2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD</td>
<td>MIBTD</td>
</tr>
<tr>
<td>101</td>
<td>1.70E-1</td>
<td>3.54E-2</td>
</tr>
<tr>
<td>161</td>
<td>1.14E-1</td>
<td>2.14E-2</td>
</tr>
<tr>
<td>201</td>
<td>8.82E-2</td>
<td>5.60E-3</td>
</tr>
<tr>
<td>321</td>
<td>6.53E-2</td>
<td>2.30E-3</td>
</tr>
<tr>
<td>401</td>
<td>5.82E-2</td>
<td>1.50E-3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$N$</th>
<th>Case 3(b): $n = 1$, $m = 15$ ($L_\infty$)</th>
<th>Case 3(b): $n = 1$, $m = 15$ ($L_2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>FDTD</td>
<td>MIBTD</td>
</tr>
<tr>
<td>101</td>
<td>1.41E-1</td>
<td>7.80E-2</td>
</tr>
<tr>
<td>161</td>
<td>1.30E-1</td>
<td>2.61E-2</td>
</tr>
<tr>
<td>201</td>
<td>1.03E-1</td>
<td>6.50E-3</td>
</tr>
<tr>
<td>321</td>
<td>7.13E-2</td>
<td>5.40E-3</td>
</tr>
<tr>
<td>401</td>
<td>6.67E-2</td>
<td>2.10E-3</td>
</tr>
</tbody>
</table>

Figure 6.12: Numerical convergence tests for the bean-shaped dispersive interface problems in TE mode. Case 3(a): ($n = 3$, $m = 3$); Case 3(b): ($n = 1$, $m = 15$). In all charts, the numerical errors are plotted as dashed lines, while the least-squares fitted convergence lines are shown as solid lines.

We are only interested in the performance of our proposed method on the numerical accuracy in this example. To explore that interest, we use the MIBTD algorithm to produce reference solution at $N = 1601$ and a sufficient small $\Delta t$. We again employ the CFL stability constant $C = 0.6$ for all our mesh refinements. The $L_\infty$ and $L_2$ errors for case 3(a) and case...
3(b) along with the numerical orders are listed in Table 6.6. Clearly, the second order convergence is always obtained for these irregular interfaces by the MIBTD method. In addition, the numerical order of case 3(a) is more uniform than that of case 3(b) probably due to the effect of the curvature magnitude. The FDTD scheme again fails to restore the designed order because of the absence of the interface treatment. To have a good knowledge of the overall convergence orders of the tested schemes, we depict all their errors in Fig. 6.12. The least-square fitting again is employed to find the convergence rate. As we can see that the numerical order \( s_{L_\infty} \) for \( L_\infty \) error and \( s_{L_2} \) for \( L_2 \) error of the MIBTD method is achieved to be \( s_{L_\infty} = 2.42, s_{L_2} = 2.13 \) for case 3(a), and \( s_{L_\infty} = 2.48, s_{L_2} = 2.10 \) for case 3(b). Since the FDTD algorithm degrades the its numerical order to as low as 1 for the interface problem, its convergence rate is found to be \( s_{L_\infty} = 0.78, s_{L_2} = 0.89 \) for case 3(a), and \( s_{L_\infty} = 0.60, s_{L_2} = 0.77 \) for case 3(b). To clearly visualize the singularity change of our field solutions across the interface, we plot the MIBTD solution at grid size \( N = 321 \) in Figs. 6.13 and 6.14. As expected, \( H_z \) solutions is not smooth when crossing the interface, and \( E_x \) and \( E_y \) still remain discontinuous.

### 6.4 Conclusion

In this work, the Debye-dispersive interface problems governed by TE mode is studied by using the matched interface time-domain (MIBTD) for the first time in the literature. Our proposed method always achieves the second-order accuracy even when dealing with the highly complex interfaces. As expected, the classical finite-difference time-domain (FDTD) without a proper interface treatment fails to restore the designed order.

In order to track the changes of the singularities of the electromagnetic field solutions, we constructed a number of the interface auxiliary differential equations (IADEs) to keep us updated the information of the jump conditions after each time step. Unlike our previous algorithms in Chapters 4 and 5, the formulations for the IADEs in this study are quite intricate due to the involvement of different fields in the staggered lattice. Therefore, to
Figure 6.13: The MIBTD solution with $N = 321$ at $t = 110$ ps for the Case 3(a) with parameters $(n,m) = (3,3)$ in TE mode. (a) Contour plot of $H_z$. (b) $H_z(16.41,y)$. (c) Contour plot of $E_y$. (d) $E_y(x,9.66)$. (e) Contour plot of $E_x$. (f) $E_x(18.56,y)$. 

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Figure 6.14: The MIBTD solution with $N = 321$ at $t = 110$ ps for the Case 3(b) with parameters $(n, m) = (1, 15)$ in TE mode. (a) Contour plot of $H_z$. (b) $H_z(x, 15)$. (c) Contour plot of $E_y$. (d) $E_y(x, 15)$. (e) Contour plot of $E_x$. (f) $E_x(17.34, y)$. 

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allow one to gain the jump condition information for the MIB treatment in dealing with the interfaces having the large curvature, a fully one-sided extrapolation scheme is proposed to discretize the IADEs with a desired accuracy. As a result, a sophisticated code is written to successfully and flexibility model the dispersive interface problems in the TE mode.

To validate the accuracy, convergence and robustness of the MIBTD method, numerous numerical studies are presented. Different complex interfaces consisting of circular, $n$–leaf rose, and bean-shaped interfaces are investigated. The numerical results reveal that our MIBTD algorithm is a second-order method, while the FDTD degrades its numerical order to 1. Additionally, the stability condition of the MIBTD method is almost the same to that of the FDTD scheme when number of grid points become large. Concerning the execution time, the MIBTD method runs about 2.14 times slower than the FDTD method. However, if a specific precision is aimed, our proposed method is more cost-effective than its counterpart because the MIBTD algorithm only makes the use of a much coarse grid.
Chapter 7

PERFECTLY MATCHED LAYER BOUNDARY CONDITIONS FOR MAXWELL INTERFACE PROBLEMS

7.1 Introduction

A highly effective absorbing boundary condition (ABC) was proposed by Berenger in 1994 [51]. In that paper, he called his new ABC perfectly matched layer (PML). This novel ABC, a nonphysical lossy medium placed and adjacent to the interested computational domain, can absorb incident waves of arbitrary angles of incidence and different frequencies. In his approach, each vector field component is split into two orthogonal components, and Maxwell’s curl equations is also appropriately split to carry out the arisen splitting-fields. To successfully derive a PML, the parameters of lossy medium are chosen based on the matching condition so that the reflection coefficient is reduced to 0.

In previous chapters 4, 5, and 6, our simulations have to be stopped before the reflected waves hit the boundaries of the computational domain because the boundary conditions of those cases are not designed to absorb the transmitted waves. Due to the interest of conducting simulations of the dispersive-interface problems in a longer time, this chapter will investigate the effectiveness of the use of the Berenger’s PML (BPML) for our concerned problems.

7.2 Modification of Maxwell’s equations in BPML

We here consider the modified Maxwell’s equations in BPML for TM\textsubscript{z} mode, and one can get field-splitting equations for TE\textsubscript{z} mode in a same manner. In BPML, $E_{z}$ is split into
\( E_{zx} \) and \( E_{zy} \) satisfying condition \( E_{z} = E_{zx} + E_{zy} \); as a result, Maxwell’s equations (2.1.18) in source-free region can be rewritten as follows

\[
\begin{align*}
\mu_2 \frac{\partial H_x}{\partial t} + \sigma^* H_x &= -\frac{\partial E_z}{\partial y} \quad (7.2.1) \\
\mu_2 \frac{\partial H_y}{\partial t} + \sigma^* H_y &= \frac{\partial E_z}{\partial x} \quad (7.2.2) \\
\epsilon_2 \frac{\partial E_{zx}}{\partial t} + \sigma_x E_{zx} &= \frac{\partial H_y}{\partial x} \quad (7.2.3) \\
\epsilon_2 \frac{\partial E_{zy}}{\partial t} + \sigma_y E_{zy} &= -\frac{\partial H_x}{\partial y} \quad (7.2.4)
\end{align*}
\]

where \( \epsilon_2 \) and \( \mu_2 \) are, respectively, electrical permittivity and magnetic permeability. In addition, \( \sigma_x \) and \( \sigma_y \) denote the electric conductivities, and \( \sigma^*_x \) and \( \sigma^*_y \) denote magnetic losses.

The choice of the parameters in the absorbing region will allow us to absorb the interested incident waves. Firstly, to satisfy the matching conditions, one can choose \( \epsilon_2 = \epsilon_1, \mu_2 = \mu_1, \) and \( \sigma_w/\epsilon_1 = \sigma^*_w/\mu_1 \) (\( w = x, y \)), in which \( \epsilon_1 \) and \( \mu_1 \) are electric and magnetic parameters of the truncated domain [51]. Moreover, to absorb the field components \((E_{zx}, H_y)\) propagating along \( x \)-direction but do not absorb the field components \((E_{zy}, H_x)\) propagating along \( y \)-direction, one must choose \((\sigma_x, \sigma^*_x, \sigma_y, \sigma^*_y) = (\sigma, \sigma^*, 0, 0)\), and note that \( \sigma \) and \( \sigma^* \) are non-zero values [51]. Similarly, to absorb waves \((E_{zy}, H_x)\) but do not absorb waves \((E_{zx}, H_y)\) the parameter set \((\sigma_x, \sigma^*_x, \sigma_y, \sigma^*_y)\) is assigned to be \((0, 0, \sigma, \sigma^*)\) [51]. To have a complete knowledge in the choice of parameter set \((\sigma_x, \sigma^*_x, \sigma_y, \sigma^*_y)\) for the PML, one can refer to Fig. 7.1. It is noted that, the discretization of the Eqs. (7.2.1),(7.2.2), (7.2.3), and (7.2.4) can be conducted in the same manner as of Maxwell system in the interested domain.

### 7.3 Grading the PML

Since the waves coming into the PML will be terminated by the outer boundary condition (BC), usually assumed to be PEC, one will expect the reflected waves coming back from that outer BC into the computational space, see Fig. 7.2. Based on that observation, the reflection error of the incident wave propagating at angle \( \theta \), traveling through the PML slab...
Figure 7.1: The parameter setting for the PML ABC.

Figure 7.2: The illustration of the waves re-entering the computational space from the outer BC.

of thickness $d$ with the left side placed at $x = 0$ is evaluated as

$$R(\theta) = e^{-2\eta \cos \theta \sigma}, \quad (7.3.1)$$
in which \( \eta = \mu / \epsilon \) is wave impedance.

In the continuous space, there is no reflection wave at a PML interface. However, in the discrete space, since conductivities \( \sigma \) and \( \sigma^* \) are discontinuous at that interface, discretizing Maxwell’s equations under those parameter settings will produce the considerable reflection wave at the PML surface. To lessen that error, the conductivity parameters in the PML slab should gradually increase from 0 to \( \sigma = \sigma_{\text{max}} \) [51]. As a result, the conductivity \( \sigma \) is now a function of \( x \) varying between 0 and \( \sigma_{\text{max}} \), and the reflection factor in the continuous world (7.3.1) becomes

\[
R(\theta) = e^{-2\eta \cos \theta \int_0^d \sigma(x) dx}.
\] (7.3.2)

In [51], Berenger proposed the polynomial grading for conductivity profile \( \sigma(x) \) as

\[
\sigma(x) = \left( \frac{x}{d} \right)^m \sigma_{\text{max}},
\] (7.3.3)

where \( m \) is a grading order, and its optimal value is often in the interval \( 3 \leq m \leq 4 \) [43]. By considering profile \( \sigma(x) \) defined in (7.3.3), the reflection error (7.3.2) will be simplified as

\[
R(\theta) = e^{-2\eta \sigma_{\text{max}} d \cos \theta (m+1)}.
\] (7.3.4)

When the thickness of the PML \( d \) is fixed, the desired reflection error \( R(0) \) and grading order \( m \) are known, the maximum value of the conductivity \( \sigma_{\text{max}} \) is given by

\[
\sigma_{\text{max}} = \frac{-(m+1) \ln |R(0)|}{2\eta d}.
\] (7.3.5)

Based on Berenger’s suggestion in his paper [51], we here will demonstrate how to evaluate \( \sigma(x) \) on the discrete grid in TM \( z \) mode along the \( x \)-line, another direction and mode will be conducted in the same way. Along the horizontal direction, only waves \( (E_{zx}, H_y) \) will be absorbed, therefore the conductivity parameters \( \sigma(x) \) and \( \sigma^*(x) \) involving in those fields will be non-zero. In the staggered grid, let assume that the front-PML interface is placed at grid
index \( L = 0 \), and PEC is placed at grid index \( L = N \), see Fig. 7.3. Therefore, the thickness of the PML is \( d = N\Delta x \). The conductivity at the grid index \( L \) is determined as an average value of cell around that index location, and given by

\[
\sigma(L) = \frac{1}{\Delta x} \int_{(L-\frac{1}{2})\Delta x}^{(L+\frac{1}{2})\Delta x} \sigma(t)dt, \quad (7.3.6)
\]

where \( \Delta x \) is the spatial increment for \( x \)-line. Note that when \( L = 0 \), the formulation (7.3.6) has the following form

\[
\sigma(0) = \frac{1}{\Delta x} \int_{0}^{\Delta x} \sigma(t)dt. \quad (7.3.7)
\]

Substituting \( \sigma(t) \) in (7.3.7) by polynomial grading (7.3.3) to achieve

\[
\sigma(0) = \frac{\sigma_{\text{max}}}{(m + 1)2^{m+1}N}. \quad (7.3.8)
\]

From (7.3.6) and (7.3.8), one can easily get the value of conductivity at grid location \( L > 0 \) as the following

\[
\sigma(L) = \sigma(0) \left[ \left(2L + 1\right)^{(m+1)} - \left(2L - 1\right)^{(m+1)} \right]. \quad (7.3.9)
\]
7.4 Numerical experiments

In this section, we conduct the simulations of Debye-interface problems in TM and TE modes, and Drude-interface problems in TM mode. To illustrate the effective of the use of PML, the stopping time is chosen to be large enough so that if the PML ABC is not applied, we will have significantly reflected waves re-entering the computational space. In all cases, the mesh size of the interested domain is $201 \times 201$, the interface of circular shape is considered for all material interfaces. The parameter settings of materials are chosen to be the same as of the dispersive-interface problems discussed in the previous chapters.

In our numerical experiments, at the time $T \leq T_1$, the left boundary of the computed space is carried out by the incident wave, the outer bottom and top boundaries are also imposed by the incident wave. But the right side of the truncated domain is placed by the PML slab, and PEC is used as the boundary condition of the outer right boundary. For $T > T_1$, the interested space is now surrounded by the PML ABC. The wave solutions are terminated at the outer left and right sides by PEC, and the outer bottom and top boundaries are assigned by the periodical BC. The choice of $T_1$ and the stopping time $T_2$ varies in different dispersive-interface problems. Specifically, in Debye-interface problems in TM and TE modes, $T_1$ and $T_2$ are, respectively, assigned to be 110 ps and 310 ps. In Drude-interface problems, $T_1 = 13.40$ fs, $T_2 = 35$ fs. In all our simulations, we use 5-cell PML ABC with grading order $m = 3$ and reflection error $R(0) = e^{-8}$. To validate the performance of BPML, we investigate the global and point errors defined as the following

$$ R(t) = 20 \log_{10} \frac{\max |u(t) - u_h(t)|}{\max |u(t)|}, \quad R^{(x,y)}(t) = 20 \log_{10} \frac{|u(x,y,t) - u_h(x,y,t)|}{\max |u(t)|}, \quad (7.4.1) $$

where $u$ and $u_h$ are, respectively, the reference and numerical solutions. $R(t)$ is the global error at observed time $T = t$, $R^{(x,y)}(t)$ is the point error of a point located at $(x, y)$ with observed time $T = t$.

We next report global errors and point errors at $A(27 \text{ mm}, 15 \text{ mm})$ and $B(27 \text{ mm}, 27 \text{ mm})$.
Figure 7.4: Structure of material interface problems using PML. Point errors are considered at two points A and B. $\Delta$ is spacial increment. $d = 5\Delta$, Debye media: $a = 30$ mm, $b = 3$ mm, Drude media: $a = 3.5$ $\mu$m, $b = 0.35$ $\mu$m.

for Debye interface problems, at $A(3.15$ $\mu$m, $1.75$ $\mu$m) and $B(3.15$ $\mu$m, $3.15$ $\mu$m) for Drude interface problems, as shown in Fig. 7.4. To benchmark the PML performance, we use solutions generated at a dense mesh size of $551 \times 551$. All the relative errors of our cases are plotted in Fig. 7.5. Overall, the use of BPML is quite effective in absorbing the wave solutions. Fig. 7.5 reads the maximum errors of global error ($s$), point error at $A$ ($s_A$), point error at $B$ ($s_B$) for Debye interface problems in TM mode, are, respectively, -32.14 dB, -49.05 dB and -39.99 dB. In the same Debye media interface but in TE mode, we get $s = -32.15$ dB, $s_A = -56.33$ dB, and $s_B = -44.38$ dB. In Drude interface problems, we obtain larger errors than previous cases; specifically, $s = -11.42$ dB, $s_A = -34.22$ dB, and $s_B = -19.52$ dB.
Figure 7.5: Relative errors for dispersive interface problems. (a) Debye media in TM mode. (b) Debye media in TE mode. (c) Drude media in TM mode.

7.5 Conclusion

This chapter is devoted to simulating the dispersive interface problems using the Berenger’s PML. The numerical results indicate the PML ABC is useful in all cases. The relative errors of the Drude interface problems are quite bigger than the rest of cases. However, those errors can be made smaller by increasing the thickness of the PML slab. Also, the results again confirm that our MIBTD methods to deal with dispersive interfaces are stable at a long-time simulation.
Chapter 8

CONCLUSION AND FUTURE WORK

Novel finite-different time-domain (FDTD) methods based on the matched interface and boundary (MIB) schemes are introduced in this dissertation. Chapter 2 briefly discussed the Maxwell’s equations along with different types of dispersive materials. Moreover, the classical FDTD, i.e Yee scheme, is constructed in solving electromagnetic system. To model general problems, PEC condition and PML are imposed as the boundary conditions.

In Chapter 3, we proposed an effective MIBTD method to handle the dielectric interfaces with discontinuous wave solutions. It can be considered as an extension of the approach reported in [26] in solving this type of interface problems. Though the jump conditions in this case are time-independent, they couple both $x$ and $y$ directions and both magnetic components. Under the staggered grid system, this characteristic of the interface conditions produces many difficulties in employing the MIB algorithm. Therefore, a very sophisticated code is written to successfully deliver a second-order accuracy of the field solutions in solving the interface problems.

In Chapter 4, to deal with the Debye dispersive interface problems, we constructed a robust MIBTD method which can effectively incorporate the time-dependent jump conditions. To track the transient changes of the waves’ regularities, we formulate the interface auxiliary differential equations (IADEs) and a hybrid Debye-Maxwell system; thereby the jump conditions are numerically evaluated after each time step. Our method is flexible in a sense that it can be easily extended to deal with the non-constant magnetic parameter. In this case, the jump relations of different field components are mixed together. Consequently,
a novel MIB method is designed to handle this tough situation. Based on the numerical results, our scheme can produce an accurate up to sixth order for the straight interfaces. For the irregular shape interfaces including constant and non-constant curvatures, and sharp corner interfaces, the proposed scheme always retains a second-order accuracy.

In Chapter 5, the Drude model was examined. Unlike the Debye medium, the ADE of this dispersive material is a second order differential equation. Consequently, the algorithm designed for Debye interface problems cannot be directly generalized for the Drude media. This chapter features a novel Drude-Maxwell system along with vigorous IADEs to take care of the second order ADE. According to the numerical results, the method in this work is able to deliver up to sixth-order accuracy for the straight interfaces. For the more complicated interfaces like fluctuation curvatures and nonsmooth interfaces, this algorithm still successfully recover the second order of accuracy.

In Chapter 6, a new matched interface and boundary time-domain (MIBTD) method is proposed to model the transverse electric (TE) Maxwells equations in Debye dispersive media with complex interfaces. Since the jump conditions of the field components are strongly dependent on the flux densities $D_x$ and $D_y$, the standard Maxwell’s equations are taken into account instead of the hybrid system as in the TM case. To update the change of the waves’ regularities across the dispersive interface, IADEs are also formulated. However, the representations of those IADEs in the TE mode are more complex than their counterparts in TM mode since they couple different field components formed on the staggered lattice. Therefore, vigorous one-sided extrapolations are discussed so that the one-sided values in the IADEs can be approximated by nearby grid-points with a second-order accuracy. Different complex interfaces consisting of circular, n-leaf rose, and bean-shaped interfaces are considered to validate the performance of the proposed MIBTD method. In any cases, the accuracy of our method is always a second order while that of classical FDTD, i.e Yee scheme, degenerates to first order.

In Chapter 7, we conducted the simulations of the dispersive interface problems discussed
in Chapters 4, 5, and 6 with BPML taking care of the ABC. The numerical results reveal that the BPML is still very effective to our interested problems.

While the leapfrog time-stepping scheme is employed for the dispersive Maxwell system in TE mode, the fourth-order Runge-Kutta (RK4) method are carried out for the rest of cases including dielectric and TM dispersive interfaces. Regardless of the material interfaces and time-stepping schemes, our novel MIBTD methods are numerically verified to be conditional stable. CPU time of our methods are also investigated. It is obvious when our MIBTD schemes always consume more CPU time than the classical FDTD methods. However, if a high precision is required, the MIBTD algorithms are actually more cost-efficient.

Finally, it is of great interests to extend our current methods to model 3D Maxwell’s equations with dispersive interface at a second-order of accuracy. Also, the electromagnetic system involving more complex and higher order dispersive materials is current under our investigation. In addition, our future work will be aimed at the study of the other physical and biological models involving the presence of different complex materials.
REFERENCES


