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Anna Rae Kirk for the degree of Master of Science in Mathematics presented on May 24, 2011.

Title: The Implicit Derivative Matching Technique for Maxwell's Equations in Complex Heterogeneous Media

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We construct an implicit derivative matching (IDM) technique for restoring the accuracy of the Yee scheme for Maxwell's equations in dispersive media with material interfaces in one dimension. We consider media exhibiting orientational polarization, which are represented using a Debye dispersive model, examples of which are water and living tissue. The problems considered here have applications to noninvasive interrogation of complex materials, and microwave imaging of biological media, among others. The IDM technique employs fictitious points to locally modify the stencil of the Yee scheme to maintain the second order accuracy that the scheme exhibits in homogeneous media. Using numerical simulations we test the convergence of the IDM-Yee scheme and demonstrate its second order accuracy. We also discuss extensions of the IDM for modifying higher order staggered finite difference schemes for Maxwell's equations in heterogeneous dispersive media.

The Implicit Derivative Matching Technique for Maxwell's Equations in Complex Heterogeneous Media

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1. INTRODUCTION

1.1. Introduction

The simulation of electromagnetic waves is important to many areas of study. For example, in medicine, electromagnetic interrogating waves can be used to detect cancerous tumors. The tumors are found by determining the properties of the tissue using an inverse problem [3]. It is important to design a fast, efficient forward solver in an inverse problem.

In this thesis we consider Maxwell's equations in complex media that incorporate material dispersion. In particular we study dispersive models of Debye type that are used to model electromagnetic wave propagation in materials such as water and living tissue, and are based on the phenomenon of orientational polarization [2, 3]. The macroscopic polarization driven by the electric field describes the averaged behavior of the model in response to the incident electromagnetic field. We employ the auxiliary differential equation (ADE) technique for modeling a dispersive medium in which an evolution equation for the polarization field, forced by the electric field, is appended to the time dependent Maxwell's equations [3]. Finite difference methods for Debye type dispersive models are obtained by discretizing Maxwell's equations, as well as the polarization evolution equation.

In the presence of material interfaces that represent discontinuities in the material parameters, the finite difference methods lose accuracy [21]. To restore accuracy, we implement a technique called the Implicit Derivative Matching (IDM) technique. This is one technique in a class of methods that are collectively called embedded finite difference time domain (FDTD) methods [21], in which the stencil of the FDTD methods are locally modified around the interface with the goal of maintaining the accuracy that the FDTD method exhibits in homogeneous media. There are several ways in which the FDTD stencils can be modified. In the IDM technique, we ask that jump conditions requiring continuity of the field variables and their time derivatives be satisfied across material interfaces. The implementation of these jump conditions is done by the introduction of fictitious nodes and values of field variables. In a pre-processing stage we obtain representation coefficients for the fictitious values which are then used to locally modify the FDTD stencils around the interface.

The major contribution of this thesis is the extension of the IDM technique, which has been previously employed for Maxwell's equations in dielectrics [21], to complex dispersive media of Debye type. We demonstrate that this extension is not trivial and requires additional considerations that are necessitated by the presence of polarization, which is specific to dispersive media. In this thesis, the IDM technique is used to modify the second order in space and time accurate Yee scheme for Debye media so that second order accuracy is maintained in the presence of material interfaces. In addition to numerically demonstrating the effectiveness of the IDM modified Yee scheme for Debye media, the thesis concludes with a discussion of the extension of the IDM technique to higher order FDTD methods for dispersive media.

In Chapter 2, we discuss Maxwell's equations in free space and Debye media and the reduction of these equations to one dimension. We examine the Yee scheme for discretizing these equations and its properties. We also discuss the (2,4) FDTD scheme for discretizing Maxwell's equations in free space, which is second order accurate in time and fourth order in space. In Chapter 3, we present the IDM technique for dielectrics. We demonstrate how this technique is used to modify the Yee and (2,4) finite difference methods to restore the accuracy of these schemes for wave propagation in presence of material interfaces in one dimension. Finally, in Chapter 4, which is the major contribution of this thesis, we extend the IDM technique to modify the Yee scheme in Debye dispersive media. We present numerical validations of our new technique. Conclusion and future directions are presented in Chapter 5.

2. MAXWELL'S EQUATIONS AND THE YEE SCHEME

2.1. Maxwell's Equations

2.1.1 Free Space

Maxwell's equations in a free space domain, i.e. $\Omega \subset \mathbb{R}^3$, from time 0 to T are given as the following system of partial differential equations

$$\text{Faraday's Law:} \qquad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{2.1}$$

$$\text{Ampere's Law:} \qquad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J}_{c,s}, \tag{2.2}$$

$$\text{Gauss' Laws:} \qquad \nabla \cdot \mathbf{B} = 0, \tag{2.3}$$

$$\nabla \cdot \mathbf{D} = \rho, \tag{2.4}$$

where each of the fields (bold face type) are functions of time t and spatial coordinate $\mathbf{x} = (x, y, z)$. The imposed boundary and initial conditions are

$$\mathbf{E}(t, x) \times \mathbf{n} = 0, \text{ for } x \in \partial\Omega, \, t \in (0, T] \tag{2.5}$$

$$\mathbf{E}(0, x) = 0 = \mathbf{H}(0, x), \text{ for } x \in \Omega. \tag{2.6}$$

Equation (2.5) defines a perfect electric conducting boundary condition on the boundary $\partial\Omega$ of Ω. The vector $\mathbf{n}$ is the unit outward normal to the boundary $\partial\Omega$. The electric field, $\mathbf{E}$, and the magnetic field, $\mathbf{H}$, are 3D vectors with $\mathbf{E} = (E_x, E_y, E_z)$ and $\mathbf{H} = (H_x, H_y, H_z)$. The electric and magnetic flux densities are defined by the constitutive laws

$$\mathbf{D} = \epsilon_0 \mathbf{E}, \tag{2.7}$$

$$\mathbf{B} = \mu_0 \mathbf{H}, \tag{2.8}$$

where ϵ_0 is free space permittivity and and μ_0 is free space permeability (both constants). The source current and conduction current (Ohm's Law) densities are both accounted for in the term $J_{c,s} = J_s + \sigma \mathbf{E}$, where σ is the conductivity of the medium [7, 3]. Note that the focus of this thesis will be on dielectric materials, which are nonconducting, so we will have $J_c = 0$ and no free charges, i.e., $\rho = 0$. An important property of dielectrics is their ability to store electrical energy, and the permittivity of the material is a measure of this [16].

The curl of a three dimensional vector $\mathbf{V} = (V_x, V_y, V_z)^T$, denoted as $\nabla \times \mathbf{V}$, is defined as

$$\nabla \times \mathbf{V} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \\ V_x & V_y & V_z \end{vmatrix},$$

which we can expand into the vector form

$$\nabla \times \mathbf{V} = \left(\frac{\partial V_z}{\partial y} - \frac{\partial V_y}{\partial z}, \frac{\partial V_x}{\partial z} - \frac{\partial V_z}{\partial x}, \frac{\partial V_y}{\partial x} - \frac{\partial V_x}{\partial y} \right)^T. \tag{2.9}$$

The Poynting theorem for Maxwell's equations tells us that energy is conserved if we have a lossless medium (i.e. no source $\mathbf{J}$) and if we have PEC boundary conditions [4]. The theorem is stated as [4]

Theorem 2.1.1.1 (Energy Conservation)**.** *If* $\mathbf{E}$ *and* $\mathbf{H}$ *are solutions of Maxwell's equations in a lossless medium, i.e. equations* (2.1) *through* (2.4) *with* $\mathbf{J}_{c,s} = 0$*, and satisfy the PEC boundary conditions*

$$\mathbf{n} \times \mathbf{E} = 0, \ \textit{or} \ \mathbf{n} \times \mathbf{H} = 0,$$

then the energy

$$\mathcal{E}(t) = \epsilon_0 \|\mathbf{E}(t)\|_2^2 + \mu_0 \|\mathbf{H}(t)\|_2^2 \equiv \text{constant}$$

$\forall\, t > 0$ *where the* $L^2(\Omega)$ *norm is defined as*

$$\|\mathbf{u}(t)\|_2^2 = \int_\Omega |\mathbf{u}(t, z)|^2 \, \mathrm{d}z.$$

2.1.2 Debye Media

In this thesis, we are concerned with Maxwell's equations in dispersive dielectrics, specifically those represented by the Debye model [6]. A dispersive medium of Debye type is one that can be polarized by an electric field. Debye materials have orientational polarization, which means its molecules have a permanent dipole moment [6]. When an electric field is applied to a Debye medium, each entire molecule aligns itself with the field, as opposed to a displacement of the electrons or atoms alone. The canonical example of Debye media is water, and another important one is biological tissue [16].

In order to model the propagation of electromagnetic waves in Debye materials, we must account for the polarization. One approach is to model the macroscopic polarization as an average of the effects of the molecules' alignment with the electric field. Polarization may have instantaneous or delayed effects. The delayed effects are affiliated with relaxation times τ, which govern the amount of time it takes for the molecules to return to their original state after the incident electromagnetic field is removed. In Debye media, the constitutive law (2.7) becomes

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P}, \tag{2.10}$$

where $\mathbf{P}$ is the macroscopic electric polarization. We will assume no magnetic effects so that we still have $\mathbf{B} = \mu_0 \mathbf{H}$. We can write $\mathbf{P}$ as

$$\mathbf{P} = \mathbf{P}_I + \mathbf{P}_R = \epsilon_0 \chi \mathbf{E} + \mathbf{P}_R, \tag{2.11}$$

i.e., as the sum of its instantaneous and relaxation parts [3]. The susceptibility, denoted by χ, is a measure of the material's ability to be polarized by an electric field. Now, we substitute (2.11) into (2.10) to obtain the constitutive law for Debye media

$$\mathbf{D} = \epsilon_0 (1 + \chi) \mathbf{E} + \mathbf{P}_R.$$

From here on, we denote $\mathbf{P}_R$ as $\mathbf{P}$ and let $\epsilon_\infty = 1 + \chi$, where ϵ_∞ is the relative permittivity of the material at infinite frequency [3]. As mentioned above, one way to describe the behavior of the polarization is to model it as an average of effects. Thus, we define polarization as

$$\mathbf{P}(t,\mathbf{x}) = \int_0^t g(t-s,\mathbf{x})\mathbf{E}(s,\mathbf{x})\,\mathrm{d}s, \tag{2.12}$$

where g is the susceptibility kernel. Note that this is a general model for $\mathbf{P}$, so it can be used for more than orientational polarization. For the Debye model, the susceptibility kernel is

$$g(t) = \mathrm{e}^{-t/\tau}\frac{\epsilon_0(\epsilon_s-\epsilon_\infty)}{\tau}, \tag{2.13}$$

where ϵ_s is the relative static permittivity, and ϵ_∞ is the infinite frequency relative permittivity. In general, ϵ_s, ϵ_∞, and τ can vary with space or time, but here we assume they are constants. The differential form for (2.12) is obtained by using the Leibniz integral rule, which differentiates (2.12) with respect to t and substitutes in (2.13):

$$\begin{aligned}\frac{\partial\mathbf{P}}{\partial t}(t,\mathbf{x}) &= g(t-t)\mathbf{E}(t,\mathbf{x}) - 0 + \int_0^t \frac{\partial}{\partial t}(g(t-s)\mathbf{E}(s,\mathbf{x}))\,\mathrm{d}s\\ &= \frac{\epsilon_0(\epsilon_s-\epsilon_\infty)}{\tau}\mathbf{E}(t,\mathbf{x}) + \int_0^t \frac{-1}{\tau}g(t-s)\mathbf{E}(s,\mathbf{x})\,\mathrm{d}s.\end{aligned}$$

This implies

$$\tau\frac{\partial\mathbf{P}}{\partial t}(t,\mathbf{x}) = \epsilon_0(\epsilon_s-\epsilon_\infty)\mathbf{E}(t,\mathbf{x}) - \int_0^t \mathrm{e}^{-(t-s)/\tau}\frac{\epsilon_0(\epsilon_s-\epsilon_\infty)}{\tau}\mathbf{E}(s,\mathbf{x})\,\mathrm{d}s,$$

which gives us the evolution equation for the polarization as

$$\tau\frac{\partial\mathbf{P}}{\partial t}(t,\mathbf{x}) + \mathbf{P}(t,\mathbf{x}) = \epsilon_0(\epsilon_s-\epsilon_\infty)\mathbf{E}(t,\mathbf{x}). \tag{2.14}$$

Equation (2.14) is the auxiliary differential equation that we append to the system of Maxwell's equations to account for polarization, along with the revised constitutive law

$$\mathbf{D} = \epsilon_0\epsilon_\infty\mathbf{E} + \mathbf{P}. \tag{2.15}$$

2.1.3 Reduction to One Dimension

We consider the 1D case where $\mathbf{E}$ oscillates in the x-direction and $\mathbf{H}$ oscillates in the y-direction, i.e., $\mathbf{E} = E_y(t,z)\mathbf{j}$ and $\mathbf{H} = H_x(t,z)\mathbf{i}$. Here on, we denote $E_y = E$ and

$H_x = H$ to simplify notation. All fields propagate in the z-direction, thus each field is represented by a scalar-valued function [3]. The curl of a scalar is reduced to a spatial derivative with respect to z, i.e.

$$\nabla \times V = \frac{\partial V}{\partial z}\mathbf{l},$$

where $\mathbf{l}$ is a unit vector in the x direction if $\mathbf{V} = \mathbf{H}$, and $\mathbf{l}$ is a unit vector in the y direction if $\mathbf{V} = \mathbf{E}$. Then Faraday's law (2.1) becomes

$$\frac{\partial E}{\partial z} = \mu_0 \frac{\partial H}{\partial t},$$

using the constitutive law $B = \mu_0 H$. If we apply the free space constitutive law $D = \epsilon_0 E$ to Ampere's law (2.2), we obtain

$$\frac{\partial H}{\partial z} = \epsilon_0 \frac{\partial E}{\partial t} + J_s.$$

Thus, Maxwell's equations for one-dimensional free space are

$$\begin{aligned} \frac{\partial H}{\partial t} &= \frac{1}{\mu_0}\frac{\partial E}{\partial z} \\ \frac{\partial E}{\partial t} &= \frac{1}{\epsilon_0}\frac{\partial H}{\partial z} - \frac{1}{\epsilon_0} J_s. \end{aligned} \tag{2.16}$$

For one dimensional Debye media, Faraday's Law will be the same since the constitutive law for the magnetic flux density does not change from free space. However, we apply (2.15) to Ampere's law (2.2) to get

$$\frac{\partial H}{\partial z} = \epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} + \frac{\partial P}{\partial t} + J_s. \tag{2.17}$$

We also have the auxiliary differential equation for polarization P (2.14) to add to our system, which in one dimension is simply

$$\frac{\partial P}{\partial t} = \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{\tau} E - \frac{1}{\tau} P. \tag{2.18}$$

Now, we want each of the equations in our system to be in terms of only one time derivative, so we apply (2.18) to (2.17) to obtain

$$\frac{\partial H}{\partial z} = \epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} + \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{\tau} E - \frac{1}{\tau} P + J_s.$$

Thus, Maxwell's equations in 1D Debye media (after rearrangement) are

$$
\begin{aligned}
\frac{\partial H}{\partial t} &= \frac{1}{\mu_0}\frac{\partial E}{\partial z} \\
\frac{\partial E}{\partial t} &= \frac{1}{\epsilon_0\epsilon_\infty}\frac{\partial H}{\partial z} - \frac{\epsilon_q - 1}{\tau}E + \frac{1}{\epsilon_0\epsilon_\infty\tau}P - \frac{1}{\epsilon_0\epsilon_\infty}J_s \\
\frac{\partial P}{\partial t} &= \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{\tau}E - \frac{1}{\tau}P,
\end{aligned}
\tag{2.19}
$$

where $\epsilon_q = \epsilon_s/\epsilon_\infty$. Note that the perfect electric conductor (PEC) conditions on the boundary of a one dimensional domain $\Omega = [a, b]$ reduce to $E(a) = E(b) = 0$. In a lossless medium we have shown energy conservation in Theorem 2.1.1.1. In a dispersive medium such as Debye, there is loss that results in energy decay. We thus have the result

Theorem 2.1.3.1 (Energy Decay)**.** *If E and H are solutions of Maxwell's equations in Debye media* (2.19) *and satisfy the PEC boundary conditions $E = 0$ on $\partial\Omega$, then we have the energy decay*

$$\mathcal{E}(t) \leq \mathcal{E}(0)\ \forall\, t > 0,$$

where

$$\mathcal{E}(t) = \epsilon_0\epsilon_\infty\|E(t)\|_2^2 + \mu_0\|H(t)\|_2^2 + \frac{1}{\epsilon_0\epsilon_d}\|P(t)\|_2^2,$$

with the $L^2(\Omega)$ norm and inner product defined as

$$\|u(t)\|_2^2 = \int_\Omega |u(t,z)|^2\,\mathrm{d}z \text{ and } (u,v) = \int_\Omega u(t,z)v(t,z)\,\mathrm{d}z.$$

Proof. From the first equation in (2.19) we have

$$\mu_0\left(\frac{\partial H}{\partial t}, H\right) = \left(\frac{\partial E}{\partial z}, H\right). \tag{A}$$

From the second equation in (2.19) we have

$$\epsilon_0\epsilon_\infty\left(\frac{\partial E}{\partial t}, E\right) = \left(\frac{\partial H}{\partial z}, E\right) - \frac{\epsilon_0\epsilon_\infty(\epsilon_q - 1)}{\tau}(E, E) + \frac{1}{\tau}(P, E). \tag{B}$$

From the third equation in (2.19) we have

$$\frac{1}{\epsilon_0\epsilon_d}\left(\frac{\partial P}{\partial t}, P\right) = \frac{1}{\tau}(E, P) - \frac{1}{\tau\epsilon_0\epsilon_d}(P, P). \tag{C}$$

Now add together (A), (B), and (C) to get

$$\mu_0\left(\frac{\partial H}{\partial t},H\right)+\epsilon_0\epsilon_\infty\left(\frac{\partial E}{\partial t},E\right)+\frac{1}{\epsilon_0\epsilon_d}\left(\frac{\partial P}{\partial t},P\right) \tag{2.20}$$

$$=-\frac{1}{\tau}\left[\|\sqrt{\epsilon_0\epsilon_d}E\|_2^2+\|\frac{1}{\sqrt{\epsilon_0\epsilon_d}}P\|_2^2-2(P,E)\right]. \tag{2.21}$$

In the above we have used the fact that $\left(\frac{\partial E}{\partial z},H\right)=-\left(\frac{\partial H}{\partial z},E\right)$, which we can show by integration by parts as

$$\begin{aligned}\left(\frac{\partial E}{\partial z},H\right)&=\int_\Omega\frac{\partial E}{\partial z}H\,\mathrm{d}z\\&=-\int_\Omega\frac{\partial H}{\partial z}E\,\mathrm{d}z+EH\Big|_{\partial\Omega}\\&=-\left(\frac{\partial H}{\partial z},E\right)\end{aligned}$$

since $E=0$ on $\partial\Omega$. Simplifying further in (2.20), we have

$$\mu_0\left(\frac{\partial H}{\partial t},H\right)+\epsilon_0\epsilon_\infty\left(\frac{\partial E}{\partial t},E\right)+\frac{1}{\epsilon_0\epsilon_d}\left(\frac{\partial P}{\partial t},P\right)=-\frac{1}{\tau}\|\sqrt{\epsilon_0\epsilon_d}E-\frac{1}{\sqrt{\epsilon_0\epsilon_d}}P\|_2^2<0 \tag{D}$$

Note that

$$\frac{\partial}{\partial t}(H,H)=\left(\frac{\partial H}{\partial t},H\right)+\left(H,\frac{\partial H}{\partial t}\right)=2\left(\frac{\partial H}{\partial t},H\right),$$

which implies $\left(\frac{\partial H}{\partial t},H\right)=\frac{1}{2}\frac{\partial}{\partial t}\|H\|_2^2$, and similarly for E, P. Then the inequality (D) becomes

$$\frac{1}{2}\frac{\partial}{\partial t}\left[\mu_0\|H\|_2^2+\epsilon_0\epsilon_\infty\|E\|_2^2+\frac{1}{\epsilon_0\epsilon_d}\|P\|_2^2\right]=\frac{1}{2}\frac{\partial}{\partial t}\mathcal{E}(t)<0.$$

$$\implies\frac{\partial}{\partial t}\mathcal{E}(t)<0.$$

The time derivative of the energy is strictly decreasing, thus,

$$\mathcal{E}(t)<\mathcal{E}(0).$$

□

2.2. Yee Scheme for Maxwell's Equations in Free Space

We consider finite difference time domain (FDTD) methods for a forward solver of Maxwell's equations in complex dispersive media, an example of which is biological tissue. These FDTD methods are advantageous because they use a uniform grid and are explicit, which means we do not have to solve a linear system at each time step. On the other hand, FDTD methods suffer from a lack of "geometric flexibility", which means it is not easy to use these methods for complicated domains [12]. Alternatively, we could use variational methods such as the finite element (FE) method, which would be unconditionally stable, unlike the FDTD methods that are only conditionally stable [1]. However, FE methods are generally more difficult and costly to implement than an FDTD method.

We will use explicit $(2, 2m)$ schemes [3] to discretize Maxwell's equations, which are second order in time and $(2m)$th order in space. In particular, we will use the classic Yee scheme, which is (2,2), and also the (2,4) scheme. There are complications with implementing a FDTD method across material interfaces, which represent a discontinuity in the electric permittivity and the magnetic permeability. In heterogeneous media, the full accuracy of a higher order FDTD method (2nd, 4th, etc) deteriorates to essentially first order accuracy [21].

The Yee scheme is an explicit finite difference method for discretizing Maxwell's equations that is second order accurate in both time and space. Second order accuracy is achieved by staggering the electric and magnetic field grid nodes for the approximations of both the spatial and temporal derivatives [20]. Let $\Delta z > 0$ and $\Delta t > 0$ be the mesh size along the z direction and the time step size, respectively. For $n = 0, 1, ...N$ and $j = 0, 1, ..., J$ define

$$(t_n, z_j) = (n\Delta t, j\Delta z)$$
$$\left(t_{n+\frac{1}{2}}, z_{j+\frac{1}{2}}\right) = \left(\left(n + \frac{1}{2}\right)\Delta t, \left(j + \frac{1}{2}\right)\Delta z\right).$$

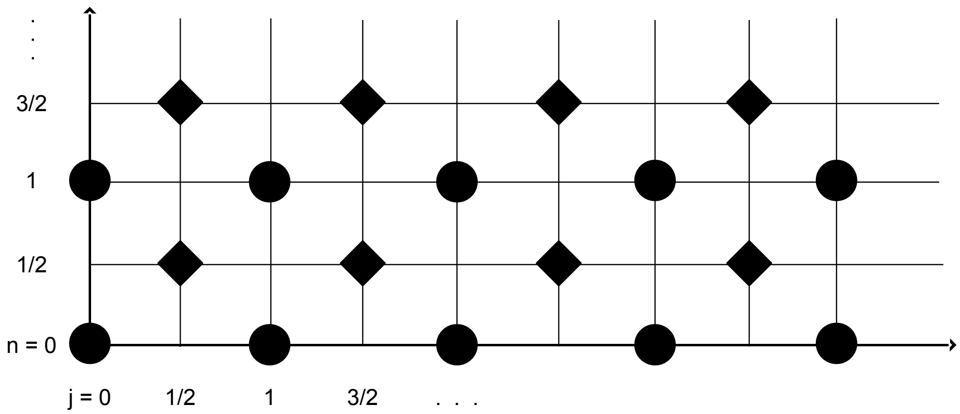


FIGURE 2.1: Staggered grid used in the Yee scheme. The horizontal axis represents space in the z direction and the vertical axis represents time. Electric field values (circles) lie on the primary grid, and magnetic field values lie on staggered grid.

The grid function E_j^n is defined on the primary grid in space-time, whereas the grid function $H_{j+\frac{1}{2}}^{n+\frac{1}{2}}$ is defined on the staggered space-time grid (see Figure 2.1). Here

$$E_j^n \approx E(t_n, z_j) \text{ and } H_{j+\frac{1}{2}}^{n+\frac{1}{2}} \approx H(t_{n+\frac{1}{2}}, z_{j+\frac{1}{2}}).$$

Figure 2.2 shows the computational stencil of the Yee scheme. The Yee scheme for free space is

$$\frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = \frac{1}{\mu_0} \frac{E_{j+1}^n - E_j^n}{\Delta z} \tag{2.22}$$

$$\frac{E_j^{n+1} - E_j^n}{\Delta t} = \frac{1}{\epsilon_0} \frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z}. \tag{2.23}$$

2.2.1 Accuracy

As mentioned above, the Yee scheme is second order accurate in both space and time. We show this is true by finding the local truncation error (LTE) of (2.22) and (2.23), denoted $(\zeta_H)_{j+\frac{1}{2}}^n$ and $(\zeta_E)_j^{n+\frac{1}{2}}$, respectively. If we substitute the exact solution into the finite difference equation written in a form that models the differential equation, which it is not expected to satisfy exactly, then the discrepancy is the LTE [13]. First

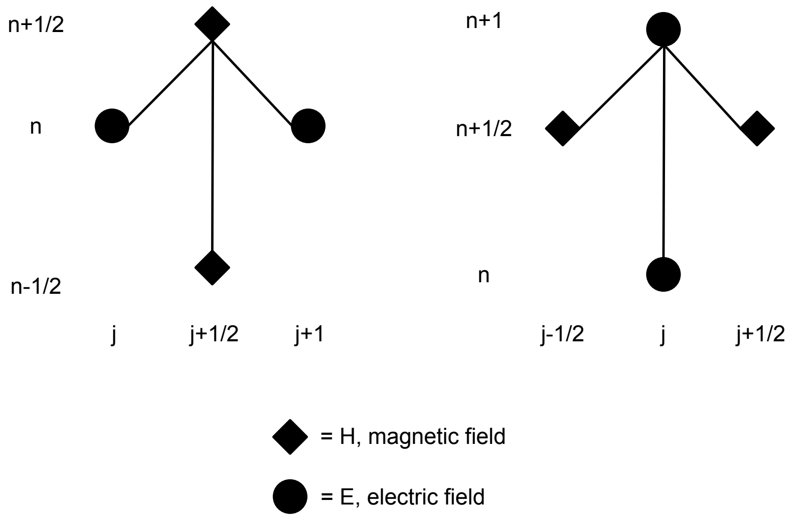


FIGURE 2.2: Stencil for the Yee scheme. The update step for the electric field grid values E_j^{n+1} depends on the previous electric field grid value E_j^n and the magnetic field grid values at a half time step before and on either side, i.e. $H_{j-\frac{1}{2}}^{n+\frac{1}{2}}$ and $H_{j+\frac{1}{2}}^{n+\frac{1}{2}}$. A similar situation holds for the update of the magnetic field at $H_{j+\frac{1}{2}}^{n+\frac{1}{2}}$.

we find $(\zeta_E)_j^{n+\frac{1}{2}}$, then $(\zeta_H)_{j+\frac{1}{2}}^n$ will follow by the same idea. The discretizations in (2.23) are centered around the point $(t_{n+\frac{1}{2}}, z_j)$, so we consider the following Taylor expansions around the same point:

$$
\begin{aligned}
E(t_{n+1}, z_j) &= E + \frac{\Delta t}{2}\frac{\partial E}{\partial t} + \frac{\Delta t^2}{8}\frac{\partial^2 E}{\partial t^2} + \frac{\Delta t^3}{48}\frac{\partial^3 E}{\partial t^3} + O(\Delta t^4) && (2.24)\\
E(t_n, z_j) &= E - \frac{\Delta t}{2}\frac{\partial E}{\partial t} + \frac{\Delta t^2}{8}\frac{\partial^2 E}{\partial t^2} - \frac{\Delta t^3}{48}\frac{\partial^3 E}{\partial t^3} + O(\Delta t^4) && (2.25)\\
H(t_{n+\frac{1}{2}}, z_{j+\frac{1}{2}}) &= H + \frac{\Delta z}{2}\frac{\partial H}{\partial z} + \frac{\Delta z^2}{8}\frac{\partial^2 H}{\partial z^2} + \frac{\Delta z^3}{48}\frac{\partial^3 H}{\partial z^3} + O(\Delta z^4) && (2.26)\\
H(t_{n+\frac{1}{2}}, z_{j-\frac{1}{2}}) &= H - \frac{\Delta z}{2}\frac{\partial H}{\partial z} + \frac{\Delta z^2}{8}\frac{\partial^2 H}{\partial z^2} - \frac{\Delta z^3}{48}\frac{\partial^3 H}{\partial z^3} + O(\Delta z^4) && (2.27)
\end{aligned}
$$

where the electric field and magnetic field terms on the right hand side are evaluated at the space-time grid point $(t_{n+\frac{1}{2}}, z_j)$. The LTE of (2.23) is

$$(\zeta_E)_j^{n+\frac{1}{2}} = \frac{E(t_{n+1}, z_j) - E(t_n, z_j)}{\Delta t} - \frac{1}{\epsilon_0}\frac{H(t_{n+\frac{1}{2}}, z_{j+\frac{1}{2}}) - H(t_{n+\frac{1}{2}}, z_{j-\frac{1}{2}})}{\Delta z}.$$

Substituting in our Taylor expansions, we have

$$
\begin{aligned}
(\zeta_E)_j^{n+\frac{1}{2}} = & \frac{1}{\Delta t}[E + \frac{\Delta t}{2}\frac{\partial E}{\partial t} + \frac{\Delta t^2}{8}\frac{\partial^2 E}{\partial t^2} + \frac{\Delta t^3}{48}\frac{\partial^3 E}{\partial t^3} + O(\Delta t^4) \\
& - (E - \frac{\Delta t}{2}\frac{\partial E}{\partial t} + \frac{\Delta t^2}{8}\frac{\partial^2 E}{\partial t^2} - \frac{\Delta t^3}{48}\frac{\partial^3 E}{\partial t^3} + O(\Delta t^4))] \\
& - \frac{1}{\epsilon_0 \Delta z}[H + \frac{\Delta z}{2}\frac{\partial H}{\partial z} + \frac{\Delta z^2}{8}\frac{\partial^2 H}{\partial z^2} + \frac{\Delta z^3}{48}\frac{\partial^3 H}{\partial z^3} + O(\Delta z^4) \\
& - (H - \frac{\Delta z}{2}\frac{\partial H}{\partial z} + \frac{\Delta z^2}{8}\frac{\partial^2 H}{\partial z^2} - \frac{\Delta z^3}{48}\frac{\partial^3 H}{\partial z^3} + O(\Delta z^4))].
\end{aligned}
$$

After cancellations, we have

$$
\begin{aligned}
(\zeta_E)_j^{n+\frac{1}{2}} &= \frac{\partial E}{\partial t} + \frac{\Delta t^2}{24}\frac{\partial^3 E}{\partial t^3} + O(\Delta t^4) - \frac{1}{\epsilon_0}\frac{\partial H}{\partial z} - \frac{\Delta z^2}{\epsilon_0 24}\frac{\partial^3 H}{\partial z^3} + O(\Delta z^4) \\
&= \frac{\Delta t^2}{24}\frac{\partial^3 E}{\partial t^3} + O(\Delta t^4) - \frac{\Delta z^2}{\epsilon_0 24}\frac{\partial^3 H}{\partial z^3} + O(\Delta z^4)
\end{aligned}
$$

Since $\frac{\partial E}{\partial t} - \frac{1}{\epsilon_0}\frac{\partial H}{\partial z} = 0$, we can see that $(\zeta_E)_j^{n+\frac{1}{2}} = O(\Delta t^2 + \Delta z^2)$. By a similar process it can be shown that the LTE of (2.22) is also $O(\Delta t^2 + \Delta z^2)$. This implies our system is second order accurate in both space and time, and we have the following lemma.

Lemma 2.2.1.1 (Truncation Error)**.** *Assume that the solutions to Maxwell's equations are smooth enough, i.e.,* $E \in C^3([0,T]; C^3(\bar{\Omega}))$ *and* $H \in C^3([0,T]; C^3(\bar{\Omega}))$*. Let* $(\zeta_E)_j^{n+\frac{1}{2}}$ *and* $(\zeta_H)_{j+\frac{1}{2}}^n$ *denote the truncation errors of the Yee scheme equations* (2.23) *and* (2.22)*, respectively. Then the truncation errors can be bounded by*

$$
\max_n \left\{ \left|(\zeta_E)_j^{n+\frac{1}{2}}\right|, \left|(\zeta_H)_{j+\frac{1}{2}}^n\right| \right\} \le c(\epsilon_0, \mu_0)(\Delta t^2 + \Delta z^2),
$$

where $c(\epsilon_0, \mu_0)$ *is a constant independent of the mesh parameters* $\Delta t > 0$ *and* $\Delta z > 0$*.*

2.2.2 Stability Analysis

The Lax-Richtmyer Equivalence Theorem [13] gives us the requirements needed for convergence of a finite difference scheme. First we need to define the concepts of consistency and stability [17].

Definition 2.2.2.1 (Consistency)**.** *Given a partial differential equation, $Pu = f$, and a finite difference scheme, $P_{\Delta t,\Delta z}v = f$, we say that the finite difference scheme is **consistent** with the PDE if for any (sufficiently) smooth function $\phi(t, z)$*

$$P\phi - P_{\Delta t,\Delta z}\phi \to 0 \text{ as } \Delta t, \Delta z \to 0$$

the convergence being pointwise convergent at each point (t,z).

Definition 2.2.2.2 (Stability)**.** *A finite difference scheme $P_{\Delta t,\Delta z}v^n_m = 0$ for a first-order equation is **stable** in the region Λ if there is an integer J such that for any positive time T, there is a constant C_T such that*

$$\|v^n\|_{\Delta z} \leq C_T \sum_{j=0}^{J} \|v^j\|_{\Delta z}$$

for $0 \leq n\Delta t \leq T$, with $(\Delta t, \Delta z) \in \Lambda$.

Note that $\|w\|_{\Delta z}$ in Definition 2.2.2.2 is the L^2 norm of the grid function w, which is defined by

$$\|w\|_{\Delta z} = \left(\Delta z \sum_{m=-\infty}^{m=\infty} |w_m|^2 \right)^{1/2} .$$

Theorem 2.2.2.1 (Lax-Richtmyer Equivalence Theorem)**.** *A consistent finite difference scheme for a partial differential equation for which the initial value problem is well-posed is convergent if and only if it is stable.*

Now that we know the importance of stability for a finite difference scheme, we will explore the stability of the Yee scheme. It is well known that the Yee scheme is conditionally stable under the necessary condition that $\nu = c\Delta t/\Delta z \leq 1$, which is called the Courant-Friedrichs-Lewy (CFL) condition. Note that $c = 1/\sqrt{\mu_0 \epsilon_0}$ is the speed of light in a vacuum and ν is called the Courant number [14, 11]. We have the following result

Theorem 2.2.2.2 (Conditional Stability of the Yee Scheme)**.** *A necessary condition for the stability of the Yee scheme* (2.22) *and* (2.23) *is the CFL condition $\nu = c\Delta t/\Delta z \leq 1$*

Proof. Assume the electric and magnetic field nodes have the spatial dependence

$$\begin{aligned} E_j^n &= \tilde{E}^n \mathrm{e}^{ikz_j}, \\ H_j^n &= \tilde{H}^n \mathrm{e}^{ikz_j}, \end{aligned} \tag{2.28}$$

where k is the wave number. We will first find the amplification matrix A such that the Yee system (2.22), (2.23) can be written in the form

$$\begin{bmatrix} \tilde{E}^{n+1} \\ \tilde{H}^{n+\frac{1}{2}} \end{bmatrix} = A \begin{bmatrix} \tilde{E}^{n} \\ \tilde{H}^{n-\frac{1}{2}} \end{bmatrix}.$$

First, substitute (2.28) into the Yee scheme update steps to obtain

$$\tilde{E}^{n+1}\mathrm{e}^{ikz_j} = \tilde{E}^n \mathrm{e}^{ikz_j} + \frac{\Delta t}{\epsilon_0 \Delta z}(\tilde{H}^{n+\frac{1}{2}}\mathrm{e}^{ikz_{j+\frac{1}{2}}} - \tilde{H}^{n+\frac{1}{2}}\mathrm{e}^{ikz_{j-\frac{1}{2}}}), \tag{2.29}$$

$$\tilde{H}^{n+\frac{1}{2}}\mathrm{e}^{ikz_{j+\frac{1}{2}}} = \tilde{H}^{n-\frac{1}{2}}\mathrm{e}^{ikz_{j+\frac{1}{2}}} + \frac{\Delta t}{\mu_0 \Delta z}(\tilde{E}^n \mathrm{e}^{ikz_{j+1}} - \tilde{E}^n \mathrm{e}^{ikz_j}). \tag{2.30}$$

Now divide (2.29) by $\mathrm{e}^{ikz_j} = \mathrm{e}^{ikj\Delta z}$ and (2.30) by $\mathrm{e}^{ikz_{j+\frac{1}{2}}} = \mathrm{e}^{ik(j+\frac{1}{2})\Delta z}$. Then, using Euler's identity, we have

$$\tilde{E}^{n+1} = \tilde{E}^n + \frac{\Delta t}{\epsilon_0 \Delta z}\tilde{H}^{n+\frac{1}{2}}(2i\sin(k\Delta z/2)), \tag{2.31}$$

$$\tilde{H}^{n+\frac{1}{2}} = \tilde{H}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_0 \Delta z}\tilde{E}^n(2i\sin(k\Delta z/2)). \tag{2.32}$$

Finally, substitute (2.32) into (2.31), which gives

$$\tilde{E}^{n+1} = \tilde{E}^n \left(1 - 4\left(\frac{c\Delta t}{\Delta z}\right)^2 \sin^2\left(\frac{k\Delta z}{2}\right)\right) + \tilde{H}^{n-\frac{1}{2}}\left(2i\frac{\Delta t}{\epsilon_0 \Delta z}\sin\left(\frac{k\Delta z}{2}\right)\right). \tag{2.33}$$

Then our matrix A from (2.32) and (2.33) is

$$A = \begin{bmatrix} 1 - 4(\frac{c\Delta t}{\Delta z})^2 \sin^2\left(\frac{k\Delta z}{2}\right) & 2i\frac{\Delta t}{\epsilon_0 \Delta z}\sin\left(\frac{k\Delta z}{2}\right) \\ 2i\frac{\Delta t}{\mu_0 \Delta z}\sin\left(\frac{k\Delta z}{2}\right) & 1 \end{bmatrix}.$$

A necessary condition for stability is that all the eigenvalues of the amplification matrix A must be less than or equal to one in magnitude. This is called the von Neumann condition

[17]. The eigenvalues of A are

$$\lambda_1 = 1 - 2\beta^2 + 2\beta\sqrt{\beta^2 - 1}$$
$$\lambda_2 = 1 - 2\beta^2 - 2\beta\sqrt{\beta^2 - 1},$$

where $\beta = \nu \sin\left(\frac{k\Delta z}{2}\right)$. First assume that $0 < \nu \leq 1$, which implies $\beta \leq 1$ and then $\sqrt{\beta^2 - 1}$ is complex. Then we can express the eigenvalues as

$$\lambda_{1,2} = 1 - 2\beta^2 \pm 2i\beta\sqrt{1 - \beta^2},$$

where $\beta\sqrt{1 - \beta^2}$ is a real number. Then we have

$$|\lambda_{1,2}|^2 = (1 - 2\beta^2)^2 + \left(2\beta\sqrt{1 - \beta^2}\right)^2 = 1,$$

so that the von Neumann condition is satisfied.

Next, assume that $\nu > 1$. By letting $\sin\left(\frac{k\Delta z}{2}\right) = 1$ we have $\beta^2 > 1$. In this case $|\lambda_2| > 1$, and the Yee scheme is unstable. $\square$

It can be shown that the condition $0 < \nu < 1$ is both necessary and sufficient for stability. However, $\nu \leq 1$ is not sufficient for stability because the Yee scheme can be unstable when $\nu = 1$ [14]. The value of the Courant number $\nu = 1$ is called the Magic Time Step, because if Δt satisfies $\nu = c\Delta t/\Delta z = 1$ and you have exact data at time step n, then the Yee scheme will produce exact data at the next time step $n + 1$ [18].

2.2.3 Dispersion Analysis

Dispersion is defined as the variation of a propagating wave's speed with frequency f [18]. A dispersive equation admits plane wave solutions of the form $e^{i(kz-\omega t)}$, where $\omega = 2\pi f$ is the angular frequency, f is the frequency in Hz, and $k = 2\pi/\lambda$ is the wavenumber. Furthermore, there exists a relationship between these quantities of the form $\omega = \omega(k)$ called the dispersion relation. A wave of this form propagates at the speed $\omega(k)/k$ called the phase velocity. When a partial differential equation is discretized, the discrete model will be dispersive, regardless of whether the continuous equation was or not [19]. Thus, in order for the numerical simulation to be successful, the continuous and numerical dispersion relations need to be "similar". We will now find the dispersion relations for the continuous and numerical versions of Maxwell's equations in one dimensional free space.

First assume we have plane wave solutions $E = E_0 \mathrm{e}^{i(kz-\omega t)}$ and $H = H_0 \mathrm{e}^{i(kz-\omega t)}$ and substitute into Maxwell's equations for free space in one-dimension (2.16). Note that the time derivative satisfies the equation $\frac{\partial E}{\partial t} = i\omega E$ and the spatial derivative satisfies $\frac{\partial E}{\partial z} = -ikE$, and similarly for H. Then Maxwell's equations transform to the equations

$$
\begin{aligned}
i\omega E_0 \mathrm{e}^{i(kz-\omega t)} &= \frac{-ik}{\epsilon_0} H_0 \mathrm{e}^{i(kz-\omega t)}, \\
i\omega H_0 \mathrm{e}^{i(kz-\omega t)} &= \frac{-ik}{\mu_0} E_0 \mathrm{e}^{i(kz-\omega t)},
\end{aligned}
$$

which we can simplify to

$$
\begin{aligned}
\omega E_0 &= \frac{-k}{\epsilon_0} H_0, \\
\omega H_0 &= \frac{-k}{\mu_0} E_0.
\end{aligned}
$$

Combining the above two equations we have

$$
\begin{aligned}
E_0 &= \frac{-k}{\omega\epsilon_0} H_0 = \frac{-\omega\mu_0}{k} H_0 \\
\Longrightarrow k^2 &= \omega^2 \epsilon_0 \mu_0 = \frac{\omega^2}{c^2} \\
\Longrightarrow k &= \frac{\omega}{c}.
\end{aligned}
\tag{2.34}
$$

Thus, the dispersion relation for Maxwell's equations in one dimensional free space is $\omega = kc$. Note that the phase velocity is $\omega/k = c$, which is a constant, so the continuous equations are dispersionless [18].

For the numerical case, we similarly assume $E_j^n = E_0 \mathrm{e}^{i(kj\Delta z - \omega n \Delta t)}$ and $H_j^n = H_0 \mathrm{e}^{i(kj\Delta z - \omega n \Delta t)}$ and substitute these into the Yee scheme (2.23), and simplify this expression by dividing by $\mathrm{e}^{i(kj\Delta z-\omega(n+\frac{1}{2})\Delta t)}$ to get

$$\frac{E_0}{\Delta t}\left(\mathrm{e}^{-i(\omega\Delta t/2)}-\mathrm{e}^{i(\omega\Delta t/2)}\right)=\frac{H_0}{\epsilon_0\Delta z}\left(\mathrm{e}^{i(k\Delta z/2)}-\mathrm{e}^{-i(k\Delta z/2)}\right).$$

Using Euler's formula $\mathrm{e}^{ix}=\cos(x)+i\sin(x)$ we get

$$\frac{E_0}{\Delta t}\left(-\sin\left(\frac{\omega\Delta t}{2}\right)\right)=\frac{H_0}{\epsilon_0\Delta z}\left(\sin\left(\frac{k\Delta z}{2}\right)\right).$$

We can do the same process for equation (2.22) and we obtain

$$\frac{H_0}{\Delta t}\left(-\sin\left(\frac{\omega\Delta t}{2}\right)\right)=\frac{E_0}{\mu_0\Delta z}\left(\sin\left(\frac{k\Delta z}{2}\right)\right).$$

Finally, combining the two equations gives us

$$\sin^2\left(\frac{\omega\Delta t}{2}\right)=\frac{\Delta t^2}{\epsilon_0\mu_0\Delta z^2}\sin^2\left(\frac{k\Delta z}{2}\right)=\nu^2\sin^2\left(\frac{k\Delta z}{2}\right).$$

Thus, the dispersion relation for the Yee scheme in one dimensional free space is

$$\sin\left(\frac{\omega\Delta t}{2}\right)=\nu\sin\left(\frac{k\Delta z}{2}\right). \tag{2.35}$$

2.2.4 Numerical Experiments

A scaled numerical example was tested for the Yee scheme in free space with the following parameter values

$$\begin{aligned}
&t\in[0,1],\quad z\in[0,1]\\
&\epsilon_0=1.0,\quad \mu_0=1.0 \implies c=1/\sqrt{\epsilon_0\mu_0}=1\\
&\frac{c\Delta t}{\Delta z}=0.9\\
&k=1 \implies \omega=ck=c=1,
\end{aligned}$$

and given the initial conditions

$$\begin{aligned}
E_j^0&=\sin(\pi k z_j),\\
H_{j+\frac{1}{2}}^{\frac{1}{2}}&=\sin\left(\frac{\pi\omega\Delta t}{2}\right)\cos\left(\pi k z_{j+\frac{1}{2}}\right),
\end{aligned}$$

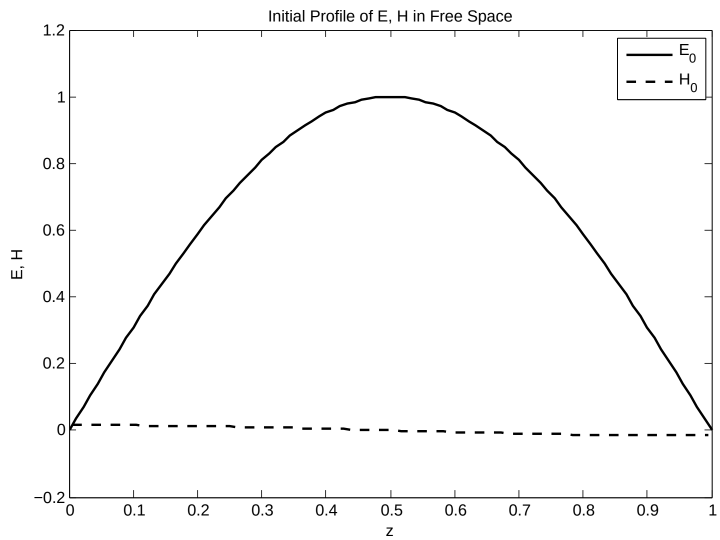


FIGURE 2.3: Initial profile of the exact solution for E, H in free space.

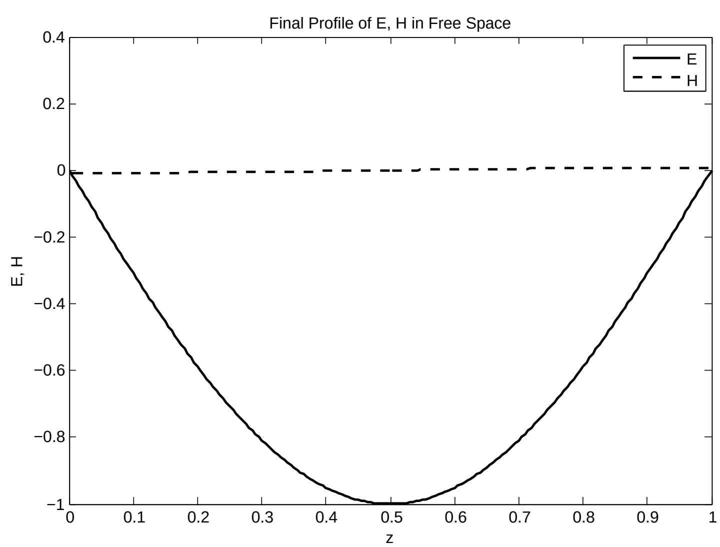


FIGURE 2.4: Final profile for E, H at time $t = 1$ in free space after the Yee scheme is applied.

TABLE 2.1: Relative error in the energy norm for the Yee Scheme in free space with varying spatial step size. The Courant number $\nu = \frac{c\Delta t}{\Delta z}$ is fixed at 0.9.

Δz	**Rel. Error**	**ratio**	**rate**
0.02	9.8892e-05	-	-
0.01	2.4523e-05	4.0327	2.0117
0.005	6.1306e-06	4	2
0.0025	1.5326e-06	4	2

for each z_j, $z_{j+\frac{1}{2}}$ in the domain. Figure 2.3 depicts the initial profile and Figure 2.4 shows the final profile of E and H. Table 2.1 shows how decreasing step size Δt by half, while maintaining the Courant number $\nu = \frac{c\Delta t}{\Delta z} = 0.9$, gives an error ratio that converges to 4. This means the numerical approximation is second order accurate as predicted. The error used was the relative error in the energy norm, which is defined in free space as

$$\mathcal{E}(t) = \int_\Omega \left(|E(t,z)|^2 + |H(t,z)|^2\right) dz = \left\|E(t,z)\right\|_2^2 + \left\|H(t,z)\right\|_2^2.$$

2.3. Yee Scheme for Maxwell's Equations in Debye Media

Recall Maxwell's equations in one dimensional Debye media (2.19). Using time step $\Delta t > 0$ and mesh step size $\Delta z > 0$, the Yee scheme for this system is

$$\frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} = \frac{1}{\mu_0}\frac{E_{j+1}^n - E_j^n}{\Delta z}, \tag{2.36a}$$

$$\frac{E_j^{n+1} - E_j^n}{\Delta t} = \frac{1}{\epsilon_0\epsilon_\infty}\frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}}{\Delta z} - \frac{\epsilon_q - 1}{\tau}\frac{E_j^{n+1} + E_j^n}{2} + \frac{1}{\epsilon_0\epsilon_\infty\tau}\frac{P_j^{n+1} + P_j^n}{2}, \tag{2.36b}$$

$$\frac{P_j^{n+1} - P_j^n}{\Delta t} = \frac{\epsilon_0(\epsilon_s - \epsilon_\infty)}{\tau}\frac{E_j^{n+1} + E_j^n}{2} - \frac{1}{\tau}\frac{P_j^{n+1} + P_j^n}{2}. \tag{2.36c}$$

Note that E, P are averaged around the point $(z_j, t_{n+\frac{1}{2}})$. This allows us to keep second order accuracy, which is proved using the same method as for free space. Also note that P is defined on the same grid points as E since they are related by the constitutive law (2.15).

As written, equations (2.36b) and (2.36c) both require knowledge of E_j^{n+1} and P_j^{n+1}, so to get proper update steps, we will take out the dependence on P_j^{n+1} in (2.36b). To do this, we simply solve (2.36c) for P_j^{n+1}, which is

$$P_j^{n+1} = \frac{\epsilon_0 \epsilon_d h_\tau}{1+h_\tau}(E_j^{n+1} + E_j^n) + \frac{1-h_\tau}{1+h_\tau} P_j^n, \tag{2.37}$$

where $h_\tau = \Delta t/2\tau$ and $\epsilon_d = \epsilon_s - \epsilon_\infty$. Now substitute this into (2.36b) and simplify to get

$$\frac{\epsilon_0(\epsilon_\infty + \epsilon_s h_\tau)}{1+h_\tau} E_j^{n+1} = \frac{\Delta t}{\Delta z}(H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}) + \frac{\epsilon_0 \epsilon_\infty (1 + 2h_\tau - \epsilon_q h_\tau)}{1+h_\tau} E_j^n + \frac{2h_\tau}{1+h_\tau} P_j^n. \tag{2.38}$$

Thus, we can write our discrete Yee system as the following explicit update steps:

$$\begin{aligned}
H_{j+\frac{1}{2}}^{n+\frac{1}{2}} &= H_{j+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_0 \Delta z}(E_{j+1}^n - E_j^n),\\
E_j^{n+1} &= \frac{1+h_\tau}{\epsilon_0(\epsilon_\infty + \epsilon_s h_\tau)}\left[\frac{\Delta t}{\Delta z}(H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}) + \frac{\epsilon_0 \epsilon_\infty (1 + 2h_\tau - \epsilon_q h_\tau)}{1+h_\tau} E_j^n + \frac{2h_\tau}{1+h_\tau} P_j^n\right],\\
P_j^{n+1} &= \frac{\epsilon_0 \epsilon_d h_\tau}{1+h_\tau}(E_j^{n+1} + E_j^n) + \frac{1-h_\tau}{1+h_\tau} P_j^n.
\end{aligned}$$

We will call this the P-formulation of the Yee scheme for Debye media. There are other equivalent ways to define the Yee scheme for Debye media. For example, the D-formulation keeps the electric flux density D in the constitutive law and eliminates P instead. The D-formulation update steps are given in [11]

$$\begin{aligned}
H_{j+\frac{1}{2}}^{n+\frac{1}{2}} &= H_{j+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_0 \Delta z}(E_{j+1}^n - E_j^n),\\
D_j^{n+1} &= D_j^n + \frac{\Delta t}{\Delta z}(H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}),\\
E_j^{n+1} &= \frac{\Delta t + 2\tau}{\eta} D_j^{n+1} + \frac{\Delta t - 2\tau}{\eta} D_j^n + \frac{\epsilon_0(2\tau\epsilon_\infty - \epsilon_s \Delta t)}{\eta} E_j^n,
\end{aligned} \tag{2.39}$$

where $\eta = \epsilon_0(2\tau\epsilon_\infty + \epsilon_s \Delta t)$. For a proof of equivalence, see [11].

2.3.1 Stability Analysis

In [3], Bokil and Gibson examine the stability of $(2, 2m)$ schemes in Debye media. They show that a necessary and sufficient condition for stability of the Yee scheme ($m = 1$) in Debye media is

$$\nu = \frac{c_\infty \Delta t}{\Delta z} < 1,$$

where $c_\infty = \dfrac{c}{\sqrt{\epsilon_\infty}}$ is the maximum speed of light in Debye media. Note that this stability condition is the same as for the Yee scheme in free space.

2.3.2 Dispersion Analysis

We begin by finding the dispersion relation for the continuous Maxwell's equations in Debye media. Similar to the free space case, we assume the fields have a plane wave solution, with the addition of $P = P_0 \mathrm{e}^{i(kz-\omega t)}$. Now substitute these into the system (2.19) to obtain

$$H_0 = \frac{-k}{\omega \mu_0} E_0, \tag{2.40a}$$

$$(-i\omega\epsilon_0\epsilon_\infty + \frac{\epsilon_0\epsilon_d}{\tau})E_0 = ikH_0 + \frac{1}{\tau}P_0, \tag{2.40b}$$

$$P_0 = \frac{\epsilon_0\epsilon_d}{1 - i\omega\tau} E_0. \tag{2.40c}$$

Now apply (2.40a) and (2.40c) to (2.40b) to get the continuous dispersion relation

$$k = \frac{\omega}{c}\sqrt{\frac{\frac{\epsilon_s}{\tau} - i\omega\epsilon_\infty}{\frac{1}{\tau} - i\omega}}.$$

Petropoulos [15] finds the numerical dispersion relation for the Yee scheme in Debye media to be

$$k_{\text{num}} = \frac{2}{\Delta z}\sin^{-1}\left[\frac{\omega}{c}\frac{\Delta z}{2} s_\omega \sqrt{\frac{\frac{\epsilon_s}{\tau}\cos(\frac{\omega\Delta t}{2}) - i\omega\epsilon_\infty s_\omega}{\frac{1}{\tau}\cos(\frac{\omega\Delta t}{2}) - i\omega s_\omega}}\right],$$

$$s_\omega = \frac{\sin(\frac{\omega\Delta t}{2})}{\frac{\omega\Delta t}{2}}.$$

As written, notice the similarities between the continuous and numerical dispersion relations. It can be shown that as $\Delta z, \Delta t$ go to zero, $k_{\text{num}} \to k$.

2.3.3 Numerical Experiments

A numerical example was tested for the Yee scheme in Debye media with the following parameter values:

$$t \in [0, 2 \times 10^{-9}], \quad z \in [0, 0.1]$$

$$\epsilon_0 = 8.85 \times 10^{-12}, \quad c = 3 \times 10^8 \text{ m/s}$$

$$\mu_0 = \frac{1}{c^2 \epsilon_0}, \quad \frac{c\Delta t}{\Delta z} = 1.0$$

$$\epsilon_s = 80.35, \quad \epsilon_\infty = 1.0, \quad \tau = 8.13 \times 10^{-12}\text{s}$$

$$k = 1 \implies \omega = ck = c$$

and zero initial conditions. The time units are in seconds. The source chosen was a truncated sine wave of the form

$$\sin\left(2\pi f\left(\left(T - \frac{1}{2}\right)\Delta t\right)\right)$$

where $f = 10^{10}$ Hz and T is the current time step. The domain was comprised of three sub-domains: first was free space, then a Debye medium, and then free space again (see Figure 2.6). The source pulse originates in free space and then moves into the Debye medium. Various values of h_τ were used (see Table 2.2), which determined the time step size, and then the spatial step size was determined using the CFL condition. Figure 2.5 shows the trace of the electric field at a point at depth 0.015 m inside the Debye medium with various time step sizes Δt. Clearly, the graphs are converging to a solution as we increase accuracy.

2.4. Fourth Order Scheme for Maxwell's Equations in Dielectrics

The explicit (2,4) scheme uses centered finite differences on a staggered grid as in the Yee scheme, but is second order accurate in time and fourth order accurate in space.

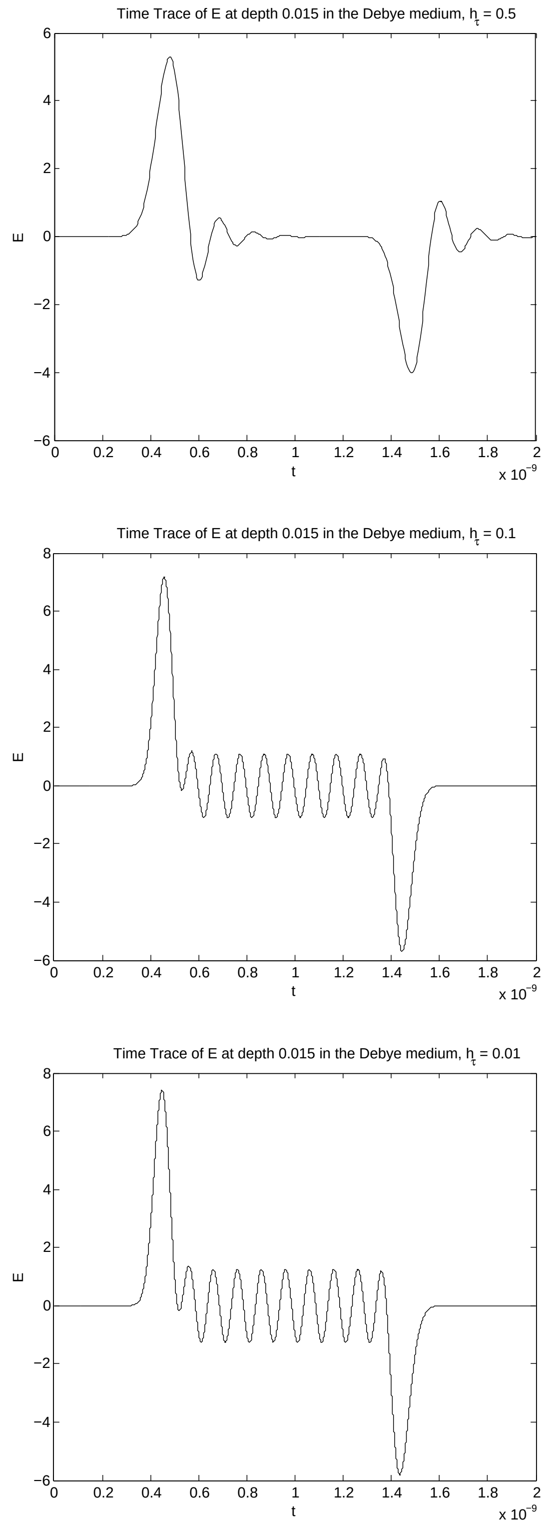


FIGURE 2.5: These graphs show the trace of the electric field over time at a point at depth 0.015m inside the Debye medium. The graphs are ordered with decreasing time step to show convergence to a solution: 0.5τ, 0.1τ, 0.01τ, where the relaxation time $\tau = 8.13 \times 10^{-12}$.

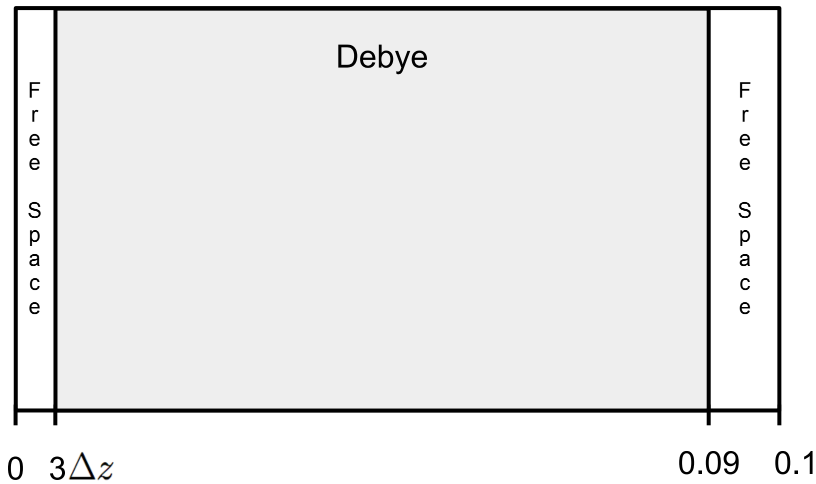


FIGURE 2.6: Domain for testing the Yee scheme in Debye media, where a source originated at $z = 0$ and then propagated into the Debye media.

TABLE 2.2: Varying values of $h_\tau = \Delta t/\tau$ determine the value of Δt, where the relaxation time $\tau = 8.13 \times 10^{-12}$. Decreasing values give a longer run time.

h_τ	Runtime (sec)
0.5	12.816002
0.1	63.612313
0.01	624.427988

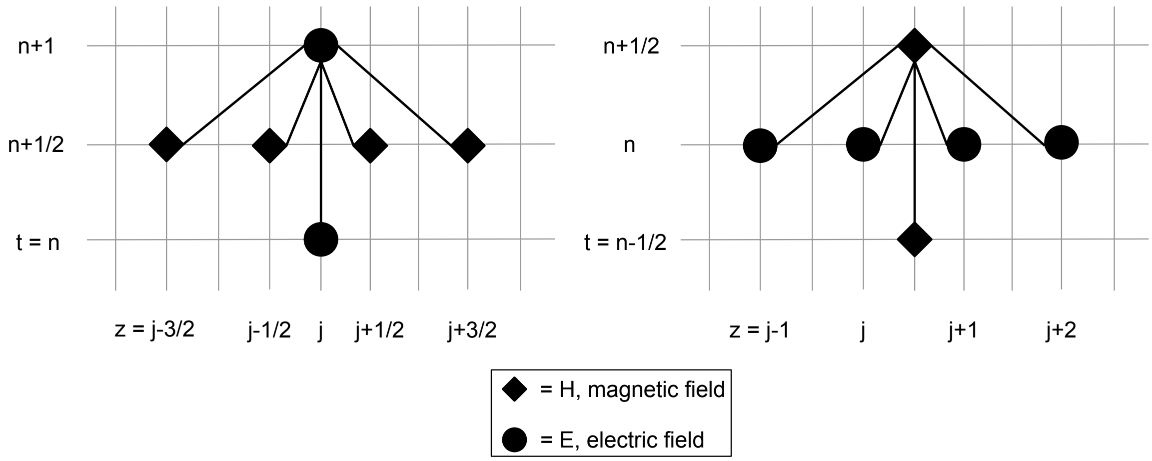


FIGURE 2.7: Stencil for the (2,4) scheme.

The scheme equations are written in the form

$$
\begin{aligned}
\frac{E_j^{n+1} - E_j^n}{\Delta t} &= \frac{1}{\epsilon_0} \frac{H_{j-\frac{3}{2}}^{n+\frac{1}{2}} - 27H_{j-\frac{1}{2}}^{n+\frac{1}{2}} + 27H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j+\frac{3}{2}}^{n+\frac{1}{2}}}{24\Delta z}, \\
\frac{H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j+\frac{1}{2}}^{n-\frac{1}{2}}}{\Delta t} &= \frac{1}{\mu_0} \frac{E_{j-1}^n - 27E_j^n + 27E_{j+1}^n - E_{j+2}^n}{24\Delta z}.
\end{aligned}
\tag{2.41}
$$

Figure 2.7 shows the computational stencil for the (2,4) scheme.

2.4.1 Boundary Conditions

Recall we assumed perfect electric conductor (PEC) boundary conditions for Maxwell's equations, which means we have

$$
E(t,a) = E(t,b) = 0 \;\forall\; t \in [0,T], \tag{2.42}
$$

in a one dimensional domain $\Omega = [a,b]$. Figure 2.8 shows that we need fictitious points outside of our domain to update the nodes closest to the boundary. We require two fictitious points for both the left and right boundaries, so we need four extra boundary conditions. We can derive these from (2.42) by applying Maxwell's equations (2.16). First apply the time derivative to (2.42)

$$
\frac{\partial E}{\partial t}(t,a) = \frac{\partial E}{\partial t}(t,b) = 0.
$$

Then by Maxwell's equations we have two new conditions on the boundary

$$\frac{\partial H}{\partial z}(t,a) = \frac{\partial H}{\partial z}(t,b) = 0. \tag{2.43}$$

Now we apply the time derivative to (2.43) to get

$$\frac{\partial}{\partial t}\frac{\partial H}{\partial z}(t,a) = \frac{\partial}{\partial t}\frac{\partial H}{\partial z}(t,b) = 0,$$

which by (2.16) is equivalent to

$$\frac{\partial^2 E}{\partial z^2}(t,a) = \frac{\partial^2 E}{\partial z^2}(t,b) = 0. \tag{2.44}$$

We need to discretize the new boundary conditions and to get representations for the fictitious points $H^{n+\frac{1}{2}}_{-\frac{1}{2}}$, $H^{n+\frac{1}{2}}_{N+\frac{1}{2}}$, E^n_{-1}, E^n_{N+1} for each $n = 0, 1, ..., N$. We use standard central differences to discretize the first and second derivatives in (2.43) and (2.44), respectively. First, we discretize (2.43) at the left boundary $z = a$ to get

$$\frac{H^{n+\frac{1}{2}}_{\frac{1}{2}} - H^{n+\frac{1}{2}}_{-\frac{1}{2}}}{2\Delta z} = 0$$

$$\implies H^{n+\frac{1}{2}}_{-\frac{1}{2}} = H^{n+\frac{1}{2}}_{\frac{1}{2}},$$

and similarly we can show that

$$H^{n+\frac{1}{2}}_{N+\frac{1}{2}} = H^{n+\frac{1}{2}}_{N-\frac{1}{2}}$$

for the right boundary. Now we discretize (2.44) at the left boundary to get

$$\frac{E^n_1 - 2E^n_0 + E^n_{-1}}{\Delta z^2} = 0. \tag{2.45}$$

Note that from equation (2.42) we have

$$E(t, z_0) = E(t, z_N) = 0 \implies E^n_0 = E^n_N = 0,$$

and applying this to (2.45) gives us

$$E^n_{-1} = -E^n_1.$$

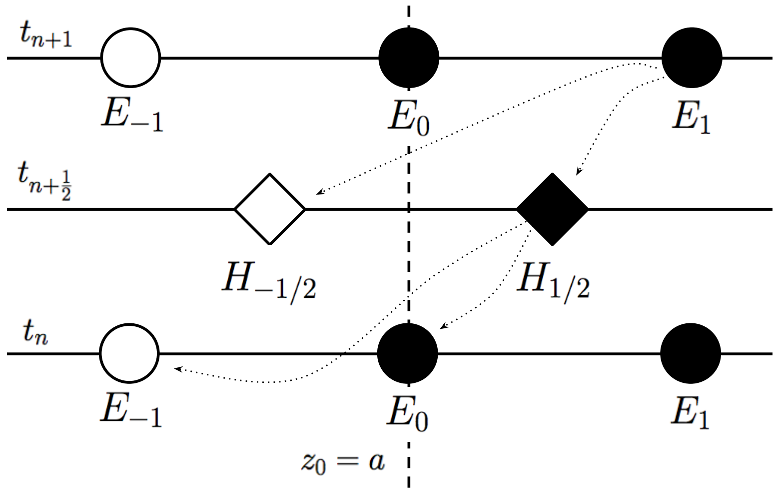


FIGURE 2.8: Layout of the grid near the left boundary of $\Omega = [a, b]$ for the (2,4) scheme. The update of $H_{\frac{1}{2}}$ and E_1 require nodes that lie outside of our domain, thus we need the fictitious points $H_{-\frac{1}{2}}$ and E_{-1}. An analogous situation takes place at the right boundary.

Similarly, we can show for the right boundary that

$$E^n_{N+1} = -E^n_{N-1}.$$

Now that we have representations for the fictitious points, we can modify the (2,4) scheme (2.41) near the boundaries to get the following update steps.

$$E^{n+1}_1 = E^n_1 + \frac{\Delta t}{24\epsilon_0 \Delta z}\left(-26H^{n+\frac{1}{2}}_{\frac{1}{2}} + 27H^{n+\frac{1}{2}}_{\frac{3}{2}} - H^{n+\frac{1}{2}}_{\frac{5}{2}}\right), \tag{2.46a}$$

$$H^{n+\frac{1}{2}}_{\frac{1}{2}} = H^{n-\frac{1}{2}}_{\frac{1}{2}} + \frac{\Delta t}{24\mu_0 \Delta z}\left(26E^n_1 - E^n_2\right), \tag{2.46b}$$

$$E^{n+1}_{N-1} = E^n_{N-1} + \frac{\Delta t}{24\epsilon_0 \Delta z}\left(H^{n+\frac{1}{2}}_{N-\frac{5}{2}} - 27H^{n+\frac{1}{2}}_{N-\frac{3}{2}} + 26H^{n+\frac{1}{2}s}_{N-\frac{1}{2}}\right), \tag{2.46c}$$

$$H^{n+\frac{1}{2}}_{N-\frac{1}{2}} = H^{n-\frac{1}{2}}_{N-\frac{1}{2}} + \frac{\Delta t}{24\mu_0 \Delta z}\left(E^n_{N-2} - 26E^n_{N-1}\right). \tag{2.46d}$$

Note that in general for a $(2, 2m)$ scheme, we would need $2m$ fictitious points outside of our domain. Therefore, we require $2m$ extra boundary conditions to find a representation of these fictitious points. If we continue the method outlined above, we would see that the boundary conditions of any order are

$$\frac{\partial^p E}{\partial z^p}(t, a) = \frac{\partial^p E}{\partial z^p}(t, b) = 0 \text{ for } p = 0, 2, 4, \ldots$$

$$\frac{\partial^p H}{\partial z^p}(t,a) = \frac{\partial^p H}{\partial z^p}(t,b) = 0 \text{ for } p = 1,3,5,\dots.$$

2.4.2 Stability Analysis

The explicit (2,4) scheme is also conditionally stable and we have the following result which is valid away from the boundaries of the domain.

Theorem 2.4.2.1 (Conditional Stability of the (2,4) Scheme)**.** *A necessary condition for stability of the explicit (2,4) scheme* (2.41) *is the CFL condition* $\nu = c\Delta t/\Delta z \leq 6/7$*.*

Proof. As before, assume the electric and magnetic field nodes have the spatial dependence.

$$\begin{aligned} E_j^n &= \tilde{E}^n \mathrm{e}^{ikz_j}, \\ H_j^n &= \tilde{H}^n \mathrm{e}^{ikz_j}. \end{aligned} \tag{2.47}$$

We will obtain the amplification matrix A such that the (2,4) system (2.41) can be written in the form

$$\begin{bmatrix} \tilde{E}^{n+1} \\ \tilde{H}^{n+\frac{1}{2}} \end{bmatrix} = A \begin{bmatrix} \tilde{E}^{n} \\ \tilde{H}^{n-\frac{1}{2}} \end{bmatrix}.$$

First, apply (2.47) to the scheme (2.41) to get

$$\begin{aligned} \tilde{E}^{n+1}\mathrm{e}^{ikz_j} &= \tilde{E}^{n}\mathrm{e}^{ikz_j} + \frac{\Delta t}{24\epsilon_0 \Delta z}\tilde{H}^{n+\frac{1}{2}}(\mathrm{e}^{ikz_{j-\frac{3}{2}}} - 27\mathrm{e}^{ikz_{j-\frac{1}{2}}} + 27\mathrm{e}^{ikz_{j+\frac{1}{2}}} - \mathrm{e}^{ikz_{j+\frac{3}{2}}}), \\ \tilde{H}^{n+\frac{1}{2}}\mathrm{e}^{ikz_{j+\frac{1}{2}}} &= \tilde{H}^{n-\frac{1}{2}}\mathrm{e}^{ikz_{j+\frac{1}{2}}} + \frac{\Delta t}{24\mu_0 \Delta z}\tilde{E}^{n}(\mathrm{e}^{ikz_{j-1}} - 27\mathrm{e}^{ikz_{j}} + 27\mathrm{e}^{ikz_{j+1}} - \mathrm{e}^{ikz_{j+2}}), \end{aligned}$$

which we can simplify by dividing by e^{ikz_j} and $\mathrm{e}^{ikz_{j+\frac{1}{2}}}$, respectively, to get

$$\tilde{E}^{n+1} = \tilde{E}^{n} + \frac{\Delta t}{24\epsilon_0 \Delta z}\tilde{H}^{n+\frac{1}{2}}(\mathrm{e}^{-3ik\Delta z/2} - 27\mathrm{e}^{-ik\Delta z/2} + 27\mathrm{e}^{ik\Delta z/2} - \mathrm{e}^{3ik\Delta z/2}), \tag{2.48}$$

$$\tilde{H}^{n+\frac{1}{2}} = \tilde{H}^{n-\frac{1}{2}} + \frac{\Delta t}{24\mu_0 \Delta z}\tilde{E}^{n}(\mathrm{e}^{-3ik\Delta z/2} - 27\mathrm{e}^{-ik\Delta z/2} + 27\mathrm{e}^{ik\Delta z/2} - \mathrm{e}^{3ik\Delta z/2}). \tag{2.49}$$

We need to take out the dependence on $\tilde{H}^{n+\frac{1}{2}}$ in equation (2.48) by substitution of (2.49), and we can also simplify the $e^{i\Delta z}$ terms. Then our system becomes

$$\begin{aligned}
\tilde{E}^{n+1} &= \tilde{E}^{n}\left[1+\left(\frac{\Delta t}{12\Delta z}\right)^2\frac{1}{\epsilon_0\mu_0}\left(27i\sin(\gamma)-i\sin(3\gamma)\right)^2\right] \\
&\quad + \tilde{H}^{n-\frac{1}{2}}\left[\frac{\Delta t}{12\epsilon_0\Delta z}\left(27i\sin(\gamma)-i\sin(3\gamma)\right)\right], \\
\tilde{H}^{n+\frac{1}{2}} &= \tilde{H}^{n-\frac{1}{2}}+\tilde{E}^{n}\left[\frac{\Delta t}{12\mu_0\Delta z}\left(27i\sin(\gamma)-i\sin(3\gamma)\right)\right],
\end{aligned}$$

where $\gamma = k\Delta z/2$. Recall the Courant number is $\nu = c\Delta t/\Delta z$, and let

$$\beta = \frac{\nu}{12}((27i\sin(\gamma)-i\sin(3\gamma)).$$

Then our matrix A is

$$A = \begin{bmatrix} 1+\beta^2 & \frac{\Delta t}{12\epsilon_0\Delta z}\left(27i\sin(\gamma)-i\sin(3\gamma)\right) \\ \frac{\Delta t}{12\mu_0\Delta z}\left(27i\sin(\gamma)-i\sin(3\gamma)\right) & 1 \end{bmatrix}$$

which has the eigenvalues

$$\lambda_{1,2} = 1+\frac{\beta^2}{2}\pm\frac{\beta}{2}\sqrt{\beta^2+4}.$$

Note that β is purely complex and so β^2 is real.

Assume that $\nu > 6/7$. By letting $\rho = 1$ we have that $\beta^2+4 < 0$. This in turn implies that $|\lambda_2| > 1$, and the von Neumann condition is not satisfied and the scheme is unstable.

Next, assume that the condition $\nu \leq 6/7$ holds. Using the triple angle formula [11] we have the relation

$$\begin{aligned}
\frac{\beta^2+4}{4} &= 1-\frac{\nu^2}{24^2}(27\sin(\gamma)-\sin(3\gamma))^2 \\
&= 1-\nu^2\rho^2\left(1+\frac{\rho^2}{6}\right)^2
\end{aligned} \tag{2.50}$$

where $\rho = \sin(k\Delta z/2)$. Since $0 \leq \rho^2 \leq 1$, we have the bound

$$\nu^2\rho^2\left(1+\frac{\rho^2}{6}\right)^2 \leq \nu^2\frac{49}{36} \leq 1 \tag{2.51}$$

TABLE 2.3: Relative error in the energy norm for the (2,4) Scheme in free space with spatial step size Δz and the Courant number $\nu = \frac{c\Delta t}{\Delta z}$ reduced by half each time. Then the time step Δt is reduced by one fourth each time so that we can see the fourth order accuracy in space.

ν	Δz	**Rel. error**	**ratio**	**rate**
0.8	0.04	0.0010262	-	-
0.4	0.02	6.4697e-05	15.862	3.9875
0.2	0.01	4.0538e-06	15.96	3.9963
0.1	0.005	2.5345e-07	15.995	3.9995
0.05	0.0025	1.5843e-08	15.998	3.9998
0.025	0.00125	9.902e-10	15.999	3.9999

Using the bound (2.51) in (2.50) we have that

$$\frac{\beta^2 + 4}{4} \geq 0. \tag{2.52}$$

This in turn implies that $|\lambda_{1,2}| = 1$, and the von Neumann condition is satisfied. As mentioned for the Yee scheme, the von Neumann condition is a necessary but not sufficient condition for stability.

$\square$

2.4.3 Numerical Experiments

To show the fourth order accuracy in space in a numerical example, we have to reduce the time step by $\frac{1}{4}$ and the space step by $\frac{1}{2}$. The same parameters and initial conditions were used as in the example in Section 2.2.4. The results of this experiment are shown in Table 2.3.

2.5. Fourth Order Scheme for Maxwell's Equations in Debye Media

A (2,4) scheme (D-formulation) is presented in [11] for Maxwell's equations in Debye media. It is similar to the D-formulation of the Yee scheme, but the second order accurate spatial derivative approximations are replaced with fourth order accurate discretizations. The explicit update steps of the scheme are [11]

$$\begin{aligned}
H_{j+\frac{1}{2}}^{n+\frac{1}{2}} &= H_{j+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{24\mu_0 \Delta z}(E_{j-1}^n - 27E_j^n + 27E_{j+1}^n - E_{j+2}^n), \\
D_j^{n+1} &= D_j^n + \frac{\Delta t}{24\Delta z}(H_{j-\frac{3}{2}}^{n+\frac{1}{2}} - 27H_{j-\frac{1}{2}}^{n+\frac{1}{2}} + 27H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j+\frac{3}{2}}^{n+\frac{1}{2}}), \\
E_j^{n+1} &= \frac{\Delta t + 2\tau}{\eta} D_j^{n+1} + \frac{\Delta t - 2\tau}{\eta} D_j^n + \frac{\epsilon_0(2\tau\epsilon_\infty - \epsilon_s \Delta t)}{\eta} E_j^n,
\end{aligned} \tag{2.53}$$

where $\eta = \epsilon_0(2\tau\epsilon_\infty + \epsilon_s\Delta t)$.

In [3], Bokil and Gibson show that the CFL condition for stability of the scheme (2.53) is $\frac{c_\infty \Delta t}{\Delta z} < \frac{6}{7}$. In addition, they analyze the dispersion relation of this scheme. This scheme is also analyzed in [11].

3. IMPLICIT DERIVATIVE MATCHING TECHNIQUE FOR (NON-DISPERSIVE) DIELECTRICS

3.1. Introduction

Finite difference methods have the advantage of being easy to implement, and in our case, the explicit schemes are also inexpensive to use. However, across material interfaces these methods lose accuracy, because of the discontinuity in the parameters defining the media [21]. We will study the implicit derivative matching (IDM) technique proposed by Zhao and Wei in [21] as a remedy to this problem. The idea of the IDM is based on ideas used by Driscoll and Fornberg in their block pseudospectral (BPS) method [9]. The BPS method, using a domain decomposition perspective, breaks the domain down into blocks and uses fictitious points to improve accuracy at the interfaces of the blocks and at the boundaries. The solution at the fictitious points is calculated at *each* time step using derivative matching conditions. However, in the IDM technique, a preprocessing scheme is used to find a representation for the solution at the fictitious points once at the beginning of the computation. Then this representation is used to locally modify the scheme near the interface, much like the embedded FDTD method [8].

3.2. Reflection-Transmission Analysis

Before we can run a simulation of the FDTD schemes in a heterogeneous material, an exact solution is needed. We use reflection-transmission analysis to develop the exact solution. The idea is that a wave incident in the first region will decompose into a transmitted wave and a reflected wave after crossing the material interface [5]. In addition, we have perfect electric conductor boundary conditions, which means any wave that reaches the boundary will be completely reflected back. Thus, the exact solution will be a combination of forward and backward moving waves in both regions of the material. With this knowledge, we can assume the following forms for E and H in the domain $\Omega = [-1, 1]$.

$$E(t,z) = \begin{cases} E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + E_1^- \mathrm{e}^{i(\omega t + k_1 z)}, & -1 \le z \le 0 \\ E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + E_2^- \mathrm{e}^{i(\omega t + k_2 z)}, & 0 \le z \le 1 \end{cases} \tag{3.1}$$

$$H(t,z) = \begin{cases} H_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + H_1^- \mathrm{e}^{i(\omega t + k_1 z)}, & -1 \le z \le 0 \\ H_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + H_2^- \mathrm{e}^{i(\omega t + k_2 z)}, & 0 \le z \le 1 \end{cases} \tag{3.2}$$

Note that $E_j^\pm$ and $H_j^\pm$ are coefficients that we need to determine, k_j is the wave number for media j, and ω is the angular frequency. The discontinuity lies in the value of the permittivity ϵ_∞, which we call ϵ_1 in medium 1 and ϵ_2 in medium 2. The magnetic permeability is constant and set to $\mu = 1$ in both media. In a dielectric, the electric constitutive law is $D = \epsilon_0 \epsilon_\infty E$ and here we are assuming $\epsilon_0 = 1$.

From Maxwell's equations (2.16), we have $\dfrac{\partial E}{\partial t} = \dfrac{1}{\epsilon}\dfrac{\partial H}{\partial z}$, where $\epsilon = \epsilon_0 \epsilon_\infty$, and with the above forms for E, H it is easy to see

$$\begin{aligned} i\omega\epsilon_1 E_1^+ &= (-ik_1) H_1^+ \implies H_1^+ = -\frac{\omega\epsilon_1}{k_1} E_1^+, \\ i\omega\epsilon_1 E_1^- &= (ik_1) H_1^- \implies H_1^- = \frac{\omega\epsilon_1}{k_1} E_1^-, \\ i\omega\epsilon_2 E_2^+ &= (-ik_2) H_2^+ \implies H_2^+ = -\frac{\omega\epsilon_2}{k_2} E_2^+, \\ i\omega\epsilon_2 E_2^- &= (ik_2) H_2^- \implies H_2^- = \frac{\omega\epsilon_2}{k_2} E_2^-. \end{aligned}$$

The dispersion relation for Maxwell's equations in dielectrics is $\omega = kc_\infty$ (recall equation (2.34)). Then we have

$$\frac{\omega\epsilon_1}{k_1} = \epsilon_1 c_1 = \sqrt{\frac{\epsilon_1}{\mu_1}} = \sqrt{\epsilon_1},$$

and similarly for medium 2. Then we can rewrite the H representation (3.2) as

$$H(t,z) = \begin{cases} -\sqrt{\epsilon_1} E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + \sqrt{\epsilon_1} E_1^- \mathrm{e}^{i(\omega t + k_1 z)}, & -1 \le z \le 0 \\ -\sqrt{\epsilon_2} E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + \sqrt{\epsilon_2} E_2^- \mathrm{e}^{i(\omega t + k_2 z)}, & 0 \le z \le 1 \end{cases} \tag{3.3}$$

Next we need to find the coefficients $E_1^+, E_1^-, E_2^+, E_2^-$. There are four constraints that our equations need to satisfy: continuity of E and H across the interface, and $E = 0$ on the boundaries. Applying the PEC boundary conditions to (3.1) gives us the following:

$$E_1^+ \mathrm{e}^{ik_1} + E_1^- \mathrm{e}^{-ik_1} = 0 \implies E_1^+ = -E_1^- \mathrm{e}^{-2ik_1}, \tag{3.4}$$

$$E_2^+ \mathrm{e}^{-ik_2} + E_2^- \mathrm{e}^{ik_2} = 0 \implies E_2^+ = -E_2^- \mathrm{e}^{2ik_2}. \tag{3.5}$$

Continuity at the interface gives us two more conditions on our coefficients

$$E_1^+ + E_1^- = E_2^+ + E_2^-, \tag{3.6}$$

$$-\sqrt{\epsilon_1} E_1^+ + \sqrt{\epsilon_1} E_1^- = -\sqrt{\epsilon_2} E_2^+ + \sqrt{\epsilon_2} E_2^-. \tag{3.7}$$

Now applying (3.4) and (3.5) to the continuity relations (3.6), (3.7) gives

$$E_1^- = E_2^- \frac{\sqrt{\epsilon_2}(1 + \mathrm{e}^{2ik_2})}{\sqrt{\epsilon_1}(1 + \mathrm{e}^{-2ik_1})}, \tag{3.8}$$

$$E_1^- = E_2^- \frac{1 - \mathrm{e}^{2ik_2}}{1 - \mathrm{e}^{-2ik_1}}. \tag{3.9}$$

There is one free parameter in the set of coefficients E_1^-, E_1^+, E_2^-, E_2^+. We choose $E_2^- = \mathrm{e}^{-i\omega(\sqrt{\epsilon_1}+\sqrt{\epsilon_2})}$ to be our free parameter. Applying this to (3.8) gives E_1^-, and subsequently, we can find E_1^+ and E_2^+ from (3.4), (3.5), respectively. Then our coefficients are

$$E_1^+ = -E_1^- \mathrm{e}^{-2i\omega\sqrt{\epsilon_1}}, \qquad E_1^- = \frac{\sqrt{\epsilon_2}\cos(\sqrt{\epsilon_2})}{\sqrt{\epsilon_1}\cos(\sqrt{\epsilon_1})},$$

$$E_2^+ = -E_2^- \mathrm{e}^{2i\omega\sqrt{\epsilon_2}}, \qquad E_2^- = \mathrm{e}^{-i\omega(\sqrt{\epsilon_1}+\sqrt{\epsilon_2})}.$$

The final thing we need is a way to calculate the angular frequency ω, which is not straightforward as in homogeneous media. In a heterogeneous dielectric, we have two wave numbers k_1, k_2 and one angular frequency ω that needs to satisfy the corresponding dispersion relations. We can relate k_1 to k_2 through (3.8) and (3.9). Then we have

$$\begin{aligned}
\frac{1-\mathrm{e}^{2ik_2}}{1-\mathrm{e}^{-2ik_1}} &= \frac{\sqrt{\epsilon_2}(1+\mathrm{e}^{2ik_2})}{\sqrt{\epsilon_1}(1+\mathrm{e}^{-2ik_1})} \\
\implies \sqrt{\epsilon_2}\frac{1+\mathrm{e}^{2ik_2}}{1-\mathrm{e}^{2ik_2}} &= \sqrt{\epsilon_1}\frac{1+\mathrm{e}^{-2ik_1}}{1-\mathrm{e}^{-2ik_1}} \\
\implies \sqrt{\epsilon_2}\frac{-\cos(k_2)}{\sin(k_2)} &= \sqrt{\epsilon_1}\frac{\cos(k_1)}{\sin(k_1)} \\
\implies -\sqrt{\epsilon_1}\tan(k_2) &= \sqrt{\epsilon_2}\tan(k_1).
\end{aligned}$$

From the dispersion relation, $k = \omega c_\infty = \omega\sqrt{\epsilon_\infty}$, since we assumed $\mu = 1$, then we have

$$-\sqrt{\epsilon_1}\tan(\omega\sqrt{\epsilon_2}) = \sqrt{\epsilon_2}\tan(\omega\sqrt{\epsilon_1}). \tag{3.10}$$

The angular frequency ω can now be found numerically from (3.10).

3.3. Numerical Test of FDTD Schemes in Heterogeneous Media

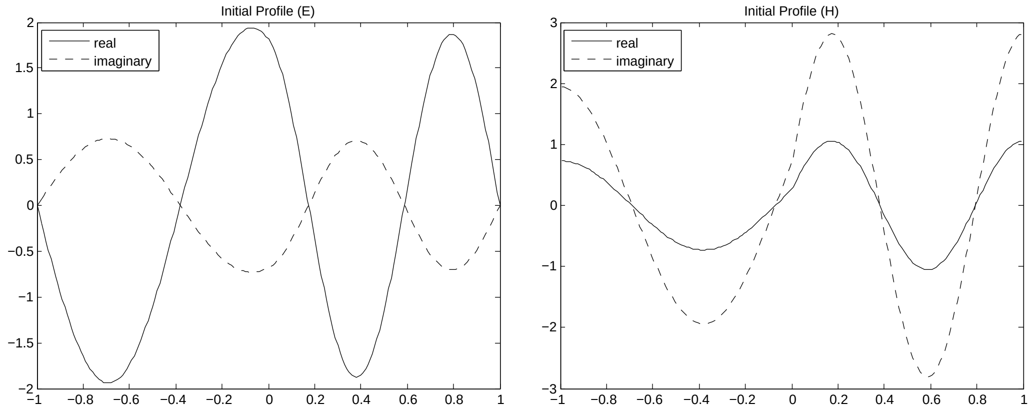
To show the loss of accuracy in FDTD schemes, we use the exact solution to Maxwell's equations that was derived in Section 3.2. for a dielectric with one interface. For this simulation, we set $\epsilon_1 = 1$ in medium 1 and $\epsilon_2 = 2.25$ in medium 2. As mentioned before, the magnetic permeability is constant and set to $\mu = 1$ and we are also assuming $\epsilon_0 = 1$. The exact solution as derived above is

$$\begin{aligned}
E(t,z) &= \begin{cases} (a_1\mathrm{e}^{i\sqrt{\epsilon_1}\omega z} - b_1\mathrm{e}^{-i\sqrt{\epsilon_1}\omega z})\mathrm{e}^{i\omega t}, & -1 \le z \le 0 \\ (a_2\mathrm{e}^{i\sqrt{\epsilon_2}\omega z} - b_2\mathrm{e}^{-i\sqrt{\epsilon_2}\omega z})\mathrm{e}^{i\omega t}, & 0 \le z \le 1 \end{cases} \\
H(t,z) &= \begin{cases} \sqrt{\epsilon_1}(a_1\mathrm{e}^{i\sqrt{\epsilon_1}\omega z} + b_1\mathrm{e}^{-i\sqrt{\epsilon_1}\omega z})\mathrm{e}^{i\omega t}, & -1 \le z \le 0 \\ \sqrt{\epsilon_2}(a_2\mathrm{e}^{i\sqrt{\epsilon_2}\omega z} + b_2\mathrm{e}^{-i\sqrt{\epsilon_2}\omega z})\mathrm{e}^{i\omega t}, & 0 \le z \le 1 \end{cases}
\end{aligned} \tag{3.11}$$

where

$$a_1 = \frac{\sqrt{\epsilon_2}\cos(\sqrt{\epsilon_2}\omega)}{\sqrt{\epsilon_1}\cos(\sqrt{\epsilon_1}\omega)}, \qquad b_1 = a_1\mathrm{e}^{-2i\sqrt{\epsilon_1}\omega},$$

$$a_2 = \mathrm{e}^{-i\omega(\sqrt{\epsilon_1}+\sqrt{\epsilon_2})}, \qquad b_2 = a_2\mathrm{e}^{2i\sqrt{\epsilon_2}\omega}.$$



(a) Electric field (b) Magnetic field

FIGURE 3.1: Initial conditions in a heterogeneous dielectric, where the interface between the two materials lies at $z = 0$.

We used the value $\omega \approx 5.07218116182516$ in our experiments [21]. Figure 3.1 plots the initial values for E and H at time $t = 0$ with the Courant number $\nu = 1.0$. Note that the solution is continuous, but not smooth across the interface at $z = 0$. To derive the accuracy of the Yee scheme, we would decrease Δt and Δz by half repeatedly. Doing this for the interface experiment gives the results in Table 3.1 and Figure 3.2. Note that the rate at which the error is converging is less than 1, indicating that the Yee scheme loses its second order accuracy in the presence of the material interface. We perform the same experiment with the (2,4) scheme and Table 3.2 and Figure 3.3 show that the accuracy is once again reduced to first order. The L^2 norm of a grid function is used to find the error at the final time $t_N = N\Delta t$, and is defined as

$$\left\| E - E_{\text{num}} \right\|_2 = \left(\Delta z \sum_{j=0}^{J} \left| E(t_N, z_j) - E_j^N \right| \right)^{1/2},$$

for the electric field error and similarly defined for the magnetic field.

TABLE 3.1: Error in L^2 norm for the Yee scheme in a dielectric with one interface. Note that the rate of convergence is approaching 1, which indicates loss of second order accuracy of the Yee scheme.

Δz	**E Error**	**ratio**	**rate**	**H Error**	**ratio**	**rate**
0.04	0.14548	-	-	0.18722	-	-
0.02	0.095679	1.5205	0.60453	0.12297	1.5225	0.60641
0.01	0.054039	1.7706	0.8242	0.069222	1.7765	0.82904
0.005	0.028484	1.8972	0.92387	0.036459	1.8986	0.92497

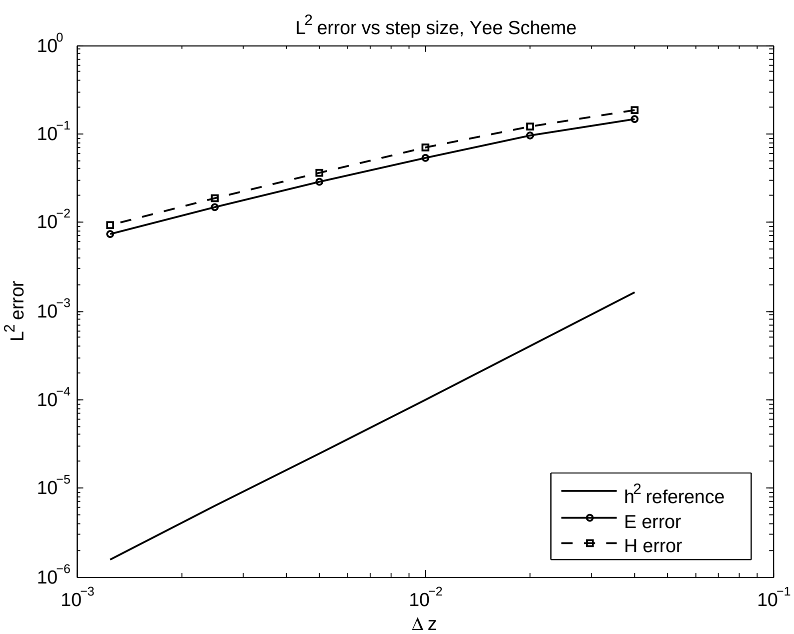


FIGURE 3.2: Log plot showing that the Yee scheme is reduced to first order accuracy in a heterogeneous dielectric material.

TABLE 3.2: Error in L^2 norm for the (2,4) scheme in a dielectric with one interface. Note that the rate of convergence is approaching 1, which indicates loss of fourth order accuracy of the (2,4) scheme.

Δz	**E error**	**ratio**	**rate**	**H error**	**ratio**	**rate**
0.04	0.2402	-	-	0.2996	-	-
0.02	0.12038	1.9953	0.99664	0.15191	1.9722	0.97984
0.01	0.06011	2.0027	1.0019	0.076442	1.9872	0.99075
0.005	0.030024	2.002	1.0015	0.038325	1.9946	0.99609

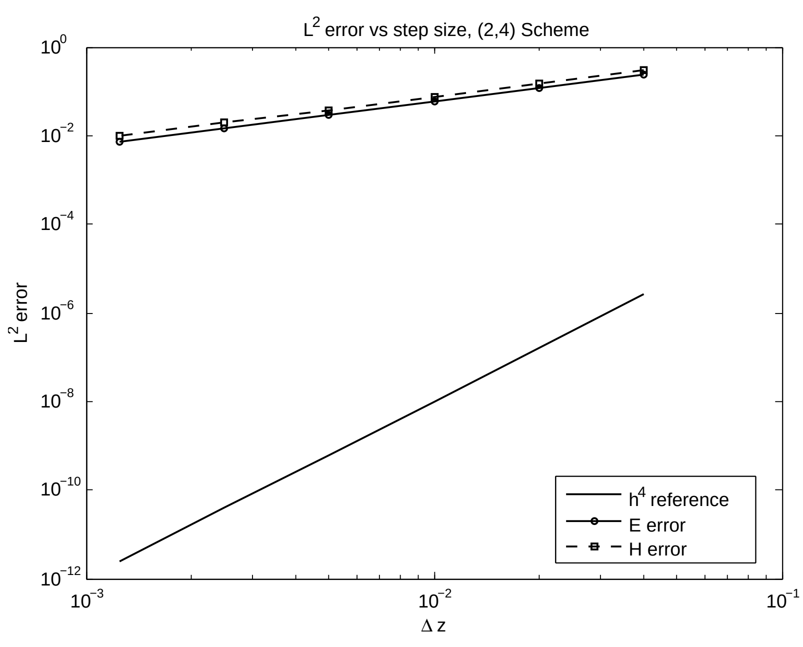


FIGURE 3.3: Log plot showing that the (2,4) scheme is reduced to first order accuracy in a heterogeneous dielectric material.

3.4. Formulation of IDM Technique

The IDM technique uses a preprocessing scheme to enforce physical jump conditions at the material interface [21]. For the moment, we will consider Maxwell's equations in dielectrics and later extend to dispersive dielectrics of Debye type in Chapter 4. Let us write the 1D Maxwell's equations (2.16) in vector form as

$$\frac{\partial \mathbf{u}}{\partial t} = A\frac{\partial \mathbf{u}}{\partial z}, \tag{3.12}$$

$$\text{with } \mathbf{u} = \begin{bmatrix} E \\ H \end{bmatrix} \text{ and } A = \begin{bmatrix} 0 & \frac{1}{\epsilon_0} \\ \frac{1}{\mu_0} & 0 \end{bmatrix}.$$

Suppose our domain has a material interface at $z = \xi$. Now we have discontinuous coefficients across the interface of our material, i.e., A takes on different values for $z < \xi$ than $z > \xi$. We denote these as A_1, A_2 for medium 1 and 2, respectively, and write this as

$$A_i = \begin{bmatrix} 0 & \frac{1}{\epsilon_i} \\ \frac{1}{\mu_i} & 0 \end{bmatrix}, \text{ for } i = 1, 2.$$

We impose the following interface conditions

$$\mathbf{n} \times (\mathbf{E}_1 - \mathbf{E}_2) = \mathbf{0}, \qquad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = 0, \tag{3.13}$$

$$\mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{0}, \qquad \mathbf{n} \cdot (\mathbf{B}_1 - \mathbf{B}_2) = 0, \tag{3.14}$$

where $\mathbf{n}$ is the unit normal vector to the interface. Note that in one dimension $\mathbf{E}_i = (0, E_i, 0)$ for $i = 1, 2$, where E_i denotes the electric field approaching from the left and right respectively, i.e.,

$$E_1 = E(t, z)\big|_{z \to \xi^-}, \; E_2 = E(t, z)\big|_{z \to \xi^+}$$

and similarly for the other fields. The interface conditions tell us that E and H are continuous across the interface, which we now show.

Let $\mathbf{n} = (0,0,1)$. Consider

$$\mathbf{n} \times (\mathbf{E}_1 - \mathbf{E}_2) = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 0 & 0 & 1 \\ 0 & E_1 - E_2 & 0 \end{vmatrix}$$

$$= -(E_1 - E_2)\mathbf{i}.$$

By the interface condition (3.13), we must have

$$E_1 - E_2 = 0 \implies E_1 = E_2.$$

This implies, $E(t,z)\big|_{z\to\xi^-} = E(t,z)\big|_{z\to\xi^+}$. Now consider

$$\mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ 0 & 0 & 1 \\ H_1 - H_2 & 0 & 0 \end{vmatrix}$$

$$= (H_1 - H_2)\mathbf{j}$$

By the interface condition (3.14), we must have

$$H_1 - H_2 = 0 \implies H_1 = H_2.$$

This implies, $H(t,z)\big|_{z\to\xi^-} = H(t,z)\big|_{z\to\xi^+}$.

The continuity relations just derived are called the zeroth order physical jump conditions, which can be expressed as

$$\mathbf{u}(t,z)\big|_{z\to\xi^-} = \mathbf{u}(t,z)\big|_{z\to\xi^+}. \tag{3.15}$$

In the IDM technique we require that $\mathbf{u}$ and its time derivatives be continuous, so Maxwell's equations can be used to show that any order derivative jump condition can be constructed. For example, taking the time derivative of the zeroth order jump condition (3.15) gives

$$\frac{\partial \mathbf{u}}{\partial t}(t,z)\big|_{z\to\xi^-} = \frac{\partial \mathbf{u}}{\partial t}(t,z)\big|_{z\to\xi^+},$$

which by the differential equation (3.12) is equivalent to

$$A_1 \frac{\partial \mathbf{u}}{\partial z}(t,z)\big|_{z\to\xi^-} = A_2 \frac{\partial \mathbf{u}}{\partial z}(t,z)\big|_{z\to\xi^+}. \tag{3.16}$$

Equation (3.16) is called the first order jump condition because it involves the first order spatial derivatives. In general, the pth-order jump condition is

$$A_1^p \mathbf{u}^{(p)}(t,\xi^-) = A_2^p \mathbf{u}^{(p)}(t,\xi^+)$$
$$\text{where } \mathbf{u}^{(p)}(t,\xi^\pm) = \frac{\partial^p \mathbf{u}}{\partial z^p}(t,z)\big|_{z\to\xi^\pm}.$$

The backbone of the IDM method is the use of fictitious points (FPs). These points are located at the same positions as E or H on the grid. We assume the representation

$$f_i = \sum_{j=1}^{2m} r_{i,j} g_j, \tag{3.17}$$

where f_i represents either an electric or magnetic fictitious point, and g_j is an actual value of either E or H depending on which we are considering. The coefficients $r_{i,j}$ are called representation coefficients. The total number of fictitious points needed to restore accuracy for the $(2, 2m)$ scheme is $2m$ (see Figure 3.4). For example, in the Yee scheme we only need $2m = 2$ fictitious points ($m = 1$) since it is second order accurate. The representation coefficients are obtained by discretizing the physical jump conditions in a preprocessing scheme as detailed below. Once we know these values, we modify the FDTD scheme using the fictitious values to calculate the update step near the interface [21].

3.5. Yee Scheme with IDM modification

In Zhao and Wei [21], the idea of the IDM technique is described for general $(2, 2m)$ schemes. The specific details for the $(2, 2)$ and $(2, 4)$ schemes were derived and implemented in this thesis.

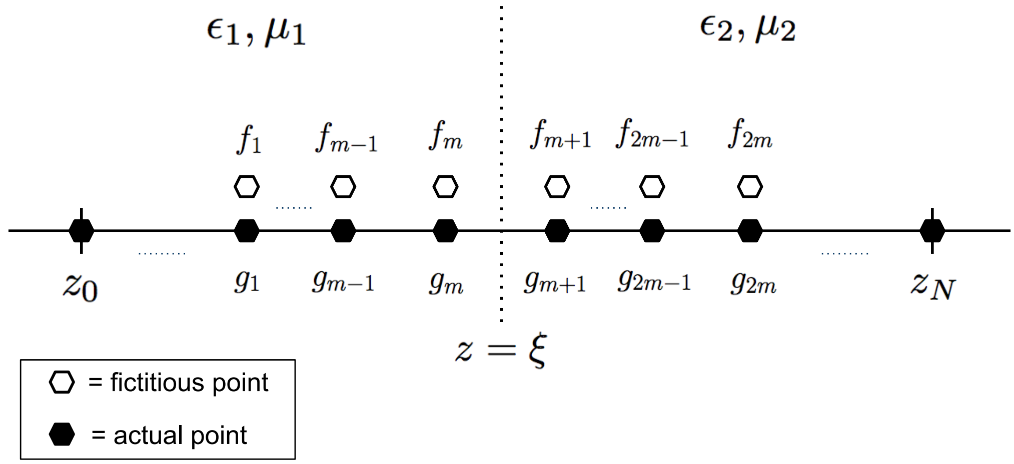


FIGURE 3.4: For a (2,2m) scheme, we use 2m fictitious points around the interface.

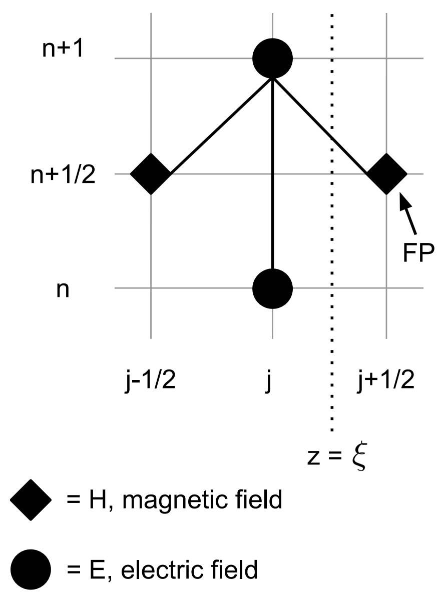


FIGURE 3.5: Stencil for the Yee scheme with an interface at $z = \xi$. Note the Yee scheme must cross the material interface to approximate E_j^{n+1}, so in the IDM method we place a fictitious point (FP) at the location of $H_{j+\frac{1}{2}}^{n+\frac{1}{2}}$. Similarly, we would need a FP at the location of E_j^n to approximate the FP at the location of $H_{j+\frac{1}{2}}^{n+\frac{1}{2}}$.

3.5.1 Representation Coefficients

Figure 3.5 gives the stencil for the update of the electric field using the Yee scheme. Note that in a material with an interface at $z = \xi$ the scheme requires an H node in medium 2 to update a E node in medium 1. To find the matrix $R = (r_{i,j})$ of $4m^2$ unknown representation coefficients, we use up to the $(2m-1)$th order jump conditions, which in the case of the Yee scheme ($m = 1$) are

$$\mathbf{u}^{(0)}(t, \xi^-) = \mathbf{u}^{(0)}(t, \xi^+) \tag{3.18}$$

$$A_1 \mathbf{u}^{(1)}(t, \xi^-) = A_2 \mathbf{u}^{(1)}(t, \xi^+). \tag{3.19}$$

The jump conditions can be approximated using the actual functional values and the fictitious values as in Figure 3.6. The finite difference weights for the spatial derivatives of different orders are calculated via the algorithm in [10]. The zeroth jump conditions are the same for E and H, so we only need to perform this approximation once. The weights for second order accuracy are $\{1/2, 1/2\}$, which gives

$$\begin{aligned} \frac{1}{2}[g_1 + f_2] &= \frac{1}{2}[f_1 + g_2] \\ \implies f_2 - f_1 &= g_2 - g_1. \end{aligned}$$

Note that $g_j = I_j G$ and $f_j = R_j G$, where I_j and R_j are the jth rows of the identity and representation matrices, respectively, and $G = [g_1, g_2]^T$. Then we have

$$\begin{aligned} (R_2 - R_1)G &= (I_2 - I_1)G \\ \implies R_2^T - R_1^T &= \begin{bmatrix} -1 \\ 1 \end{bmatrix}. \end{aligned} \tag{3.20}$$

The first order jump condition (3.19) can be represented as the system

$$\begin{aligned} \frac{1}{\mu_1} E^{(1)}(t, \xi^-) &= \frac{1}{\mu_2} E^{(1)}(t, \xi^+), \\ \frac{1}{\epsilon_1} H^{(1)}(t, \xi^-) &= \frac{1}{\epsilon_2} H^{(1)}(t, \xi^+). \end{aligned}$$

Again, we only approximate the equations once in a general form by letting $c_i = \epsilon_i$, μ_i and using the weights $\{-1/\Delta z, 1/\Delta z\}$, so we have:

$$\begin{aligned} \frac{1}{c_1}[-g_1 + f_2] &= \frac{1}{c_2}[-f_1 + g_2] \\ \Longrightarrow \frac{1}{c_2}f_1 + \frac{1}{c_1}f_2 &= \frac{1}{c_1}g_1 + \frac{1}{c_2}g_2 \\ \Longrightarrow \frac{1}{c_2}R_1^T + \frac{1}{c_1}R_2^T &= \begin{bmatrix} 1/c_1 \\ 1/c_2 \end{bmatrix}. \end{aligned} \tag{3.21}$$

Now we put together (3.20) and (3.21) to get the system

$$\begin{bmatrix} -1 & 1 \\ 1/c_2 & 1/c_1 \end{bmatrix} \begin{bmatrix} r_{1,1} & r_{1,2} \\ r_{2,1} & r_{2,2} \end{bmatrix} = \begin{bmatrix} -1 & 1 \\ 1/c_1 & 1/c_2 \end{bmatrix}.$$

We solve for the $r_{i,j}$'s and substitute in $c_i = \mu_i$ for E and $c_i = \epsilon_i$ for H to get

$$R^E = \frac{1}{\mu_1 + \mu_2} \begin{bmatrix} 2\mu_2 & \mu_1 - \mu_2 \\ \mu_2 - \mu_1 & 2\mu_1 \end{bmatrix},$$

and

$$R^H = \frac{1}{\epsilon_1 + \epsilon_2} \begin{bmatrix} 2\epsilon_2 & \epsilon_1 - \epsilon_2 \\ \epsilon_2 - \epsilon_1 & 2\epsilon_1 \end{bmatrix}.$$

3.5.2 Modification of Yee Scheme

Figure 3.6 shows the locations of the fictitious points needed for the IDM technique applied to the Yee scheme. Note that the electric field variables E_i now represent nodal values, and similarly for the other field variables. We see that E_2 depends on H_1, which lies across the material interface. Thus, we modify the Yee scheme for E_2 by using the fictitious point H_1^* in place of H_1. Note that $H_1^* = R_1^H G^H$, where R_1^H is the first row of R^H and $G^H = [H_1, H_2]^T$ is the vector of actual values. Using these facts, we can modify

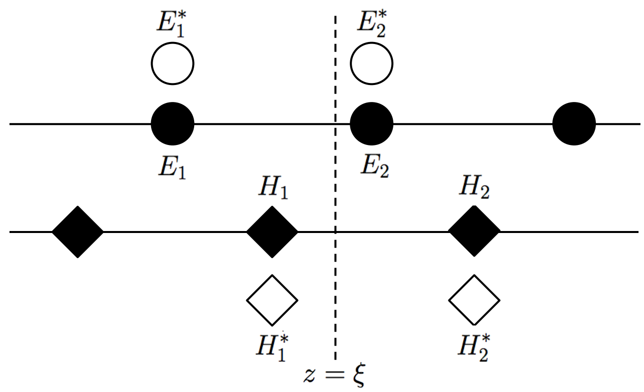


FIGURE 3.6: Layout of the grid around the material interface at $z = \xi$. The starred (*) field variables are the fictitious points, which lie at the same position as the corresponding actual points.

the Yee scheme for E_2^{n+1} (see Figure 3.6) as

$$\begin{aligned}
E_2^{n+1} &= E_2^n + \frac{\Delta t}{\epsilon_2 \Delta z}\left(H_2^{n+\frac{1}{2}} - H_1^{*\,n+\frac{1}{2}}\right) \\
&= E_2^n + \frac{\Delta t}{\epsilon_2 \Delta z}\left(H_2^{n+\frac{1}{2}} - \left(r_{11}^H H_1^{n+\frac{1}{2}} + r_{12}^H H_2^{n+\frac{1}{2}}\right)\right) \\
&= E_2^n + \frac{\Delta t}{\epsilon_2 \Delta z}\left(\left(1 - r_{12}^H\right) H_2^{n+\frac{1}{2}} - r_{11}^H H_1^{n+\frac{1}{2}}\right) \\
&= E_2^n + \frac{\Delta t}{\epsilon_2 \Delta z}\left[\left(1 - \frac{\epsilon_1 - \epsilon_2}{\epsilon_1 + \epsilon_2}\right) H_2^{n+\frac{1}{2}} - \frac{2\epsilon_2}{\epsilon_1 + \epsilon_2} H_1^{n+\frac{1}{2}}\right] \\
&= E_2^n + \frac{\Delta t}{\epsilon_2 \Delta z}\left[\frac{2\epsilon_2}{\epsilon_1 + \epsilon_2} H_2^{n+\frac{1}{2}} - \frac{2\epsilon_2}{\epsilon_1 + \epsilon_2} H_1^{n+\frac{1}{2}}\right] \\
&= E_2^n + \frac{\Delta t}{\left(\frac{\epsilon_1 + \epsilon_2}{2}\right)\Delta z}\left(H_2^{n+\frac{1}{2}} - H_1^{n+\frac{1}{2}}\right).
\end{aligned}$$

We need to do the same sort of modification for H_1 since its update requires the node E_2 that lies across the interface (see Figure 3.6). The modification of the Yee scheme for H_1 needs the fictitious point $E_2^* = R_2^E G^E$, where $G^E = [E_1,\, E_2]^T$. Using these facts we can modify the Yee scheme for $H_1^{n+\frac{1}{2}}$ (see Figure 3.6) as

$$\begin{aligned}
H_1^{n+\frac{1}{2}} &= H_1^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_1 \Delta z} \left(E_2^{*\,n} - E_1^n\right) \\
&= H_1^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_1 \Delta z} \left(r_{21}^E E_1^n + r_{22}^E E_2^n - E_1^n\right) \\
&= H_1^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_1 \Delta z} \left(\left(r_{21}^E - 1\right) E_1^n + r_{22}^E E_2^n\right) \\
&= H_1^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_1 \Delta z} \left(\left(\frac{\mu_2 - \mu_1}{\mu_2 + \mu_1} - 1\right) E_1^n + \frac{2\mu_1}{\mu_2 + \mu_1} E_2^n\right) \\
&= H_1^{n-\frac{1}{2}} + \frac{\Delta t}{\mu_1 \Delta z} \left(\frac{-2\mu_1}{\mu_2 + \mu_1} E_1^n + \frac{2\mu_1}{\mu_2 + \mu_1} E_2^n\right) \\
&= H_1^{n-\frac{1}{2}} + \frac{\Delta t}{\left(\frac{\mu_2 + \mu_1}{2}\right) \Delta z} \left(E_2^n - E_1^n\right).
\end{aligned}$$

Thus applying the IDM technique to the Yee scheme gives the following method, in which the IDM modification is to take an average of the permittivities ϵ_1, ϵ_2 near the interface, and similarly for the permeabilities μ_1, μ_2. The electric field update in the modified Yee scheme is

$$\begin{aligned}
E_i^{n+1} &= E_i^n + \frac{\Delta t}{\chi^E \Delta z} \left(H_{i+\frac{1}{2}}^{n+\frac{1}{2}} - H_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) \\
\text{where } \chi^E &= \begin{cases} \dfrac{\epsilon_1 + \epsilon_2}{2} & : \text{if } z_i \text{ nearest to interface} \\ \epsilon_1 & : z_i < \xi \\ \epsilon_2 & : z_i > \xi \end{cases}
\end{aligned}$$

while the magnetic field update in the modified Yee scheme is

$$\begin{aligned}
H_{i+\frac{1}{2}}^{n+\frac{1}{2}} &= H_{i+\frac{1}{2}}^{n-\frac{1}{2}} + \frac{\Delta t}{\chi^H \Delta z} \left(E_{i+1}^n - E_i^n\right) \\
\text{where } \chi^H &= \begin{cases} \dfrac{\mu_1 + \mu_2}{2} & : \text{if } z_{i+1/2} \text{ nearest to interface} \\ \mu_1 & : z_{i+1/2} < \xi \\ \mu_2 & : z_{i+1/2} > \xi \end{cases} .
\end{aligned}$$

3.5.3 Numerical Experiment

Recall in Section 3.3. we had an exact solution (3.11) for Maxwell's equations in a dielectric medium with an interface. We demonstrated that the accuracy of the Yee scheme was reduced to first order due to the presence of a material interface. Now we use the same initial conditions derived from (3.11) and apply the Yee scheme with IDM modification. Table 3.3 gives the results of this numerical simulation and clearly we have the second order rate of convergence restored to the modified Yee scheme. Figure 3.7 shows the second order accuracy in a log-log plot.

TABLE 3.3: Error in L^2 norm for the Yee scheme with IDM modification in a dielectric medium with one interface.

Δz	**E** L^2 **error**	**ratio**	**rate**	**H** L^2 **error**	**ratio**	**rate**
0.04	0.11038	-	-	0.13649	-	-
0.02	0.027636	3.9941	1.9979	0.03413	3.999	1.9996
0.01	0.00691	3.9994	1.9998	0.0085299	4.0012	2.0004
0.005	0.0017249	4.006	2.0021	0.0021292	4.006	2.0022

3.6. Fourth Order Scheme with IDM modification

3.6.1 Representation Coefficients

We first show how to calculate the representation matrix R^H. For the case $m = 2$, we have four magnetic field nodes to consider: H_{-2}, H_{-1}, H_1, H_2 (see Figure 3.8). The standard centered finite difference weights centered at $z = \xi$ for the derivatives indicated

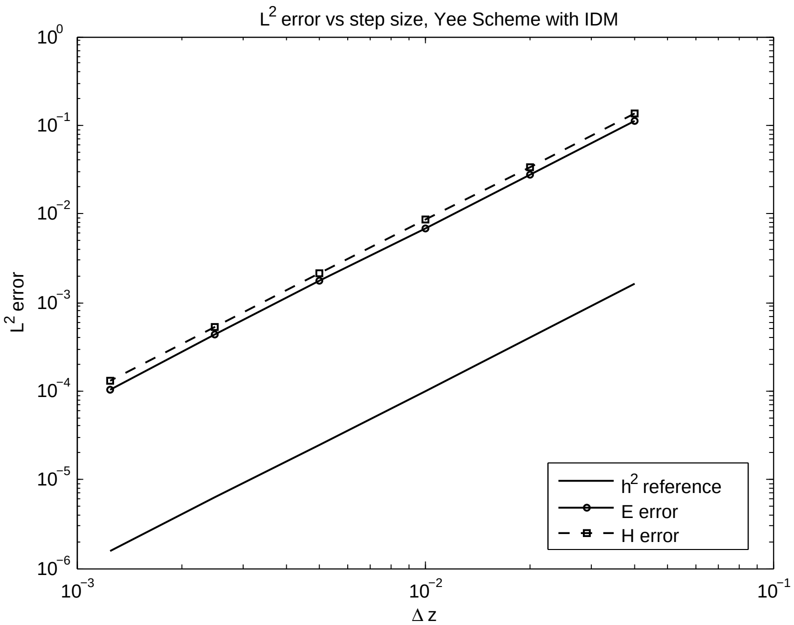


FIGURE 3.7: Log plot showing the Yee scheme with the IDM modification is second order accurate in space.

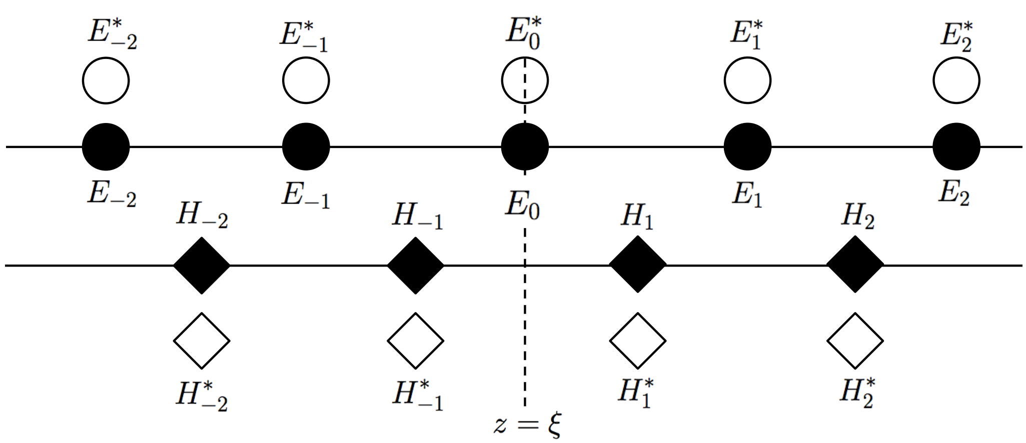


FIGURE 3.8: Layout of the grid around the material interface at $z = \xi$. The starred (*) field variables are the fictitious points, which lie at the same position as the corresponding actual points

(below) are calculated using Fornberg's algorithm in [10]

$$
\begin{array}{lcccc}
0^{\text{th}}: & \frac{-1}{16}, & \frac{9}{16}, & \frac{9}{16}, & \frac{-1}{16} \\
1^{\text{st}}: & \frac{1}{24\Delta z}, & \frac{-9}{8\Delta z}, & \frac{9}{8\Delta z}, & \frac{-1}{24\Delta z} \\
2^{\text{nd}}: & \frac{1}{2\Delta z^2}, & \frac{-1}{2\Delta z^2}, & \frac{-1}{2\Delta z^2}, & \frac{1}{2\Delta z^2} \\
3^{\text{rd}}: & \frac{-1}{\Delta z^3}, & \frac{3}{\Delta z^3}, & \frac{-3}{\Delta z^3}, & \frac{1}{\Delta z^3}
\end{array}
$$

As before, denote actual magnetic field values by g_i and fictitious points by f_i. We discretize the pth order jump conditions for H according to the weights above.

- Zeroth order jump condition: $H^{(0)}(t,\xi^-) = H^{(0)}(t,\xi^+)$. We have

$$
\begin{aligned}
&\frac{-1}{16}g_{-3/2} + \frac{9}{16}g_{-1/2} + \frac{9}{16}f_{1/2} + \frac{-1}{16}f_{3/2} = \frac{-1}{16}f_{-3/2} + \frac{9}{16}f_{-1/2} + \frac{9}{16}g_{1/2} + \frac{-1}{16}g_{3/2} \\
&\implies \frac{1}{16}\left[f_{-3/2} - 9f_{-1/2} + 9f_{1/2} - f_{3/2}\right] = \frac{1}{16}\left[g_{-3/2} - 9g_{-1/2} + 9g_{1/2} - g_{3/2}\right] \\
&\implies R_1G - 9R_2G + 9R_3G - R_4G = I_1G - 9I_2G + 9I_3G - I_4G \\
&\implies R_1^T - 9R_2^T + 9R_3^T - R_4^T = \begin{bmatrix} 1 \\ -9 \\ 9 \\ -1 \end{bmatrix}.
\end{aligned} \tag{3.22}
$$

- First order jump condition: $\dfrac{1}{\epsilon_1}H^{(1)}(t,\xi^-) = \dfrac{1}{\epsilon_2}H^{(1)}(t,\xi^+)$. We have

$$
\begin{aligned}
&\frac{1}{\epsilon_1}\left[\frac{1}{24}g_{-3/2} + \frac{-9}{8}g_{-1/2} + \frac{9}{8}f_{1/2} + \frac{-1}{24}f_{3/2}\right] \\
&\qquad = \frac{1}{\epsilon_2}\left[\frac{1}{24}f_{-3/2} + \frac{-9}{8}f_{-1/2} + \frac{9}{8}g_{1/2} + \frac{-1}{24}g_{3/2}\right] \\
&\implies \frac{1}{24}\left[\frac{-1}{\epsilon_2}f_{-3/2} + \frac{27}{\epsilon_2}f_{-1/2} + \frac{27}{\epsilon_1}f_{1/2} - \frac{1}{\epsilon_1}f_{3/2}\right] \\
&\qquad = \frac{1}{24}\left[\frac{-1}{\epsilon_1}g_{-3/2} + \frac{27}{\epsilon_1}g_{-1/2} + \frac{27}{\epsilon_2}g_{1/2} - \frac{1}{\epsilon_2}g_{3/2}\right]
\end{aligned}
$$

$$\begin{aligned}\implies \frac{-1}{\epsilon_2}R_1G + \frac{27}{\epsilon_2}R_2G + \frac{27}{\epsilon_1}R_3G + \frac{-1}{\epsilon_1}R_4G \\ = \frac{-1}{\epsilon_1}I_1G + \frac{27}{\epsilon_1}I_2G + \frac{27}{\epsilon_2}I_3G + \frac{-1}{\epsilon_2}I_4G\end{aligned}$$

$$\implies -\epsilon_1 R_1^T + 27\epsilon_1 R_2^T + 27\epsilon_2 R_3^T - \epsilon_2 R_4^T = \begin{bmatrix} -\epsilon_2 \\ 27\epsilon_2 \\ 27\epsilon_1 \\ -\epsilon_1 \end{bmatrix}. \tag{3.23}$$

- Second order jump condition: $\frac{1}{\epsilon_1\mu_1}H^{(2)}(t,\xi^-) = \frac{1}{\epsilon_2\mu_2}H^{(2)}(t,\xi^+)$. We have

$$\frac{1}{2\epsilon_1\mu_1}\left[g_{-3/2} - g_{-1/2} - f_{1/2} + f_{3/2}\right] = \frac{1}{2\epsilon_2\mu_2}\left[f_{-3/2} - f_{-1/2} - g_{1/2} + g_{3/2}\right]$$

$$\begin{aligned}\implies \frac{1}{2}\left[\frac{-1}{\epsilon_2\mu_2}f_{-3/2} + \frac{1}{\epsilon_2\mu_2}f_{-1/2} + \frac{-1}{\epsilon_1\mu_1}f_{1/2} + \frac{1}{\epsilon_1\mu_1}f_{3/2}\right] \\ = \frac{1}{2}\left[\frac{-1}{\epsilon_1\mu_1}g_{-3/2} + \frac{1}{\epsilon_1\mu_1}g_{-1/2} + \frac{-1}{\epsilon_2\mu_2}g_{1/2} + \frac{1}{\epsilon_2\mu_2}g_{3/2}\right]\end{aligned}$$

$$\begin{aligned}\implies \frac{-1}{\epsilon_2\mu_2}R_1G + \frac{1}{\epsilon_2\mu_2}R_2G + \frac{-1}{\epsilon_1\mu_1}R_3G + \frac{1}{\epsilon_1\mu_1}R_4G \\ = \frac{-1}{\epsilon_1\mu_1}I_1G + \frac{1}{\epsilon_1\mu_1}I_2G + \frac{-1}{\epsilon_2\mu_2}I_3G + \frac{1}{\epsilon_2\mu_2}I_4G\end{aligned}$$

$$\implies -\epsilon_1\mu_1 R_1^T + \epsilon_1\mu_1 R_2^T - \epsilon_2\mu_2 R_3^T + \epsilon_2\mu_2 R_4^T = \begin{bmatrix} -\epsilon_2\mu_2 \\ \epsilon_2\mu_2 \\ -\epsilon_1\mu_1 \\ \epsilon_1\mu_1 \end{bmatrix}. \tag{3.24}$$

- Third order jump condition: $\frac{1}{\epsilon_1^2\mu_1}H^{(2)}(t,\xi^-) = \frac{1}{\epsilon_2^2\mu_2}H^{(2)}(t,\xi^+)$. We have

$$\frac{1}{\epsilon_1^2\mu_1}\left[-g_{-3/2} + 3g_{-1/2} - 3f_{1/2} + f_{3/2}\right] = \frac{1}{\epsilon_2^2\mu_2}\left[-f_{-3/2} + 3f_{-1/2} - 3g_{1/2} + g_{3/2}\right]$$

$$\begin{aligned}\implies \frac{1}{\epsilon_2^2\mu_2}f_{-3/2} + \frac{-3}{\epsilon_2^2\mu_2}f_{-1/2} + \frac{-3}{\epsilon_1^2\mu_1}f_{1/2} + \frac{1}{\epsilon_1^2\mu_1}f_{3/2} \\ = \frac{1}{\epsilon_1^2\mu_1}g_{-3/2} + \frac{-3}{\epsilon_1^2\mu_1}g_{-1/2} + \frac{-3}{\epsilon_2^2\mu_2}g_{1/2} + \frac{1}{\epsilon_2^2\mu_2}g_{3/2}\end{aligned}$$

$$\Longrightarrow \frac{1}{\epsilon_2^2\mu_2}R_1G + \frac{-3}{\epsilon_2^2\mu_2}R_2G + \frac{-3}{\epsilon_1^2\mu_1}R_3G + \frac{1}{\epsilon_1^2\mu_1}R_4G$$

$$= \frac{1}{\epsilon_1^2\mu_1}I_1G + \frac{-3}{\epsilon_1^2\mu_1}I_2G + \frac{-3}{\epsilon_2^2\mu_2}I_3G + \frac{1}{\epsilon_2^2\mu_2}I_4G$$

$$\Longrightarrow \epsilon_1^2\mu_1R_1^T - 3\epsilon_1^2\mu_1R_2^T - 3\epsilon_2^2\mu_2R_3^T + \epsilon_2^2\mu_2R_4^T = \begin{bmatrix} \epsilon_2^2\mu_2 \\ -3\epsilon_2^2\mu_2 \\ -3\epsilon_1^2\mu_1 \\ \epsilon_1^2\mu_1 \end{bmatrix}. \tag{3.25}$$

Now put together the equations (3.22), (3.23), (3.24), (3.25) to get following the system for R^H

$$\begin{bmatrix} 1 & -9 & 9 & -1 \\ -\epsilon_1 & 27\epsilon_1 & 27\epsilon_2 & -\epsilon_2 \\ -\epsilon_1\mu_1 & \epsilon_1\mu_1 & -\epsilon_2\mu_2 & \epsilon_2\mu_2 \\ \epsilon_1^2\mu_1 & -3\epsilon_1^2\mu_1 & -3\epsilon_2^2\mu_2 & \epsilon_2^2\mu_2 \end{bmatrix} R^H = \begin{bmatrix} 1 & -9 & 9 & -1 \\ -\epsilon_2 & 27\epsilon_2 & 27\epsilon_1 & -\epsilon_1 \\ -\epsilon_2\mu_2 & \epsilon_2\mu_2 & -\epsilon_1\mu_1 & \epsilon_1\mu_1 \\ \epsilon_2^2\mu_2 & -3\epsilon_2^2\mu_2 & -3\epsilon_1^2\mu_1 & \epsilon_1^2\mu_1 \end{bmatrix}.$$

Next we do a similar analysis in order to find R^E. There are five electric field nodes to consider $E_{-2}, E_{-1}, E_0, E_1, E_2$ (see Figure 3.8), so we use up to the 4th order jump conditions to find the representation coefficients. The standard fourth order centered finite difference weights for the derivatives needed are

$$\begin{array}{llllll} 0^{\text{th}}: & 0, & 0, & 1, & 0, & 0 \\ 1^{\text{st}}: & \frac{1}{12\Delta z}, & \frac{-2}{3\Delta z}, & 0, & \frac{2}{3\Delta z}, & \frac{-1}{12\Delta z} \\ 2^{\text{nd}}: & \frac{-1}{12\Delta z^2}, & \frac{4}{3\Delta z^2}, & \frac{-5}{2\Delta z^2}, & \frac{4}{3\Delta z^2}, & \frac{-1}{12\Delta z^2} \\ 3^{\text{rd}}: & \frac{-1}{2\Delta z^3}, & \frac{1}{\Delta z^3}, & 0, & \frac{1}{\Delta z^3}, & \frac{1}{2\Delta z^3} \\ 4^{\text{th}}: & \frac{1}{\Delta z^4}, & \frac{-4}{\Delta z^4}, & \frac{6}{\Delta z^4}, & \frac{-4}{\Delta z^4}, & \frac{1}{\Delta z^4} \end{array}$$

- Zeroth order jump condition: $E^{(0)}(t,\xi^-) = E^{(0)}(t,\xi^+)$. We have

$$g_0 = f_0 \Longrightarrow R_3 = I_3. \tag{3.26}$$

- First order jump condition: $\dfrac{1}{\mu_1}E^{(1)}(t,\xi^-) = \dfrac{1}{\mu_2}E^{(1)}(t,\xi^+)$. We have

$$\begin{aligned}
&\frac{1}{\mu_1}\left[\frac{1}{12}g_{-2} + \frac{-2}{3}g_{-1} + 0g_0 + \frac{2}{3}f_1 - \frac{1}{12}f_2\right] \\
&\qquad\qquad = \frac{1}{\mu_2}\left[\frac{1}{12}f_{-2} + \frac{-2}{3}f_{-1} + 0g_0 + \frac{2}{3}g_1 - \frac{1}{12}g_2\right] \\
&\implies \frac{-1}{\mu_2}f_{-2} + \frac{8}{\mu_2}f_{-1} + \frac{8}{\mu_1}f_1 - \frac{1}{\mu_1}f_2 = \frac{-1}{\mu_1}g_{-2} + \frac{8}{\mu_1}g_{-1} + \frac{8}{\mu_2}g_1 - \frac{1}{\mu_2}g_2 \\
&\implies -\mu_1 R_1^T + 8\mu_1 R_2^T + 8\mu_2 R_4^T - \mu_2 R_5^T = \begin{bmatrix} -\mu_2 \\ 8\mu_2 \\ 0 \\ 8\mu_1 \\ -\mu_1 \end{bmatrix}.
\end{aligned} \tag{3.27}$$

- Second order jump condition: $\dfrac{1}{\epsilon_1\mu_1}E^{(2)}(t,\xi^-) = \dfrac{1}{\epsilon_2\mu_2}E^{(2)}(t,\xi^+)$. We have

$$\begin{aligned}
&\frac{1}{\epsilon_1\mu_1}\left[\frac{-1}{12}g_{-2} + \frac{4}{3}g_{-1} + \frac{-5}{2}g_0 + \frac{4}{3}f_1 - \frac{1}{12}f_2\right] \\
&\qquad\qquad = \frac{1}{\epsilon_2\mu_2}\left[\frac{-1}{12}f_{-2} + \frac{4}{3}f_{-1} + \frac{-5}{2}g_0 + \frac{4}{3}g_1 - \frac{-1}{12}g_2\right] \\
&\implies \frac{1}{\epsilon_2\mu_2}f_{-2} + \frac{-16}{\epsilon_2\mu_2}f_{-1} + \frac{30}{\epsilon_2\mu_2}f_0 + \frac{16}{\epsilon_1\mu_1}f_1 + \frac{-1}{\epsilon_1\mu_1}f_2 \\
&\qquad\qquad = \frac{1}{\epsilon_1\mu_1}g_{-2} + \frac{-16}{\epsilon_1\mu_1}g_{-1} + \frac{30}{\epsilon_1\mu_1}g_0 + \frac{16}{\epsilon_2\mu_2}g_1 + \frac{-1}{\epsilon_2\mu_2}g_2 \\
&\implies \epsilon_1\mu_1 R_1^T - 16\epsilon_1\mu_1 R_2^T + 30\epsilon_1\mu_1 R_3^T + 16\epsilon_2\mu_2 R_4^T - \epsilon_2\mu_2 R_5^T = \begin{bmatrix} \epsilon_2\mu_2 \\ -16\epsilon_2\mu_2 \\ 30\epsilon_2\mu_2 \\ 16\epsilon_1\mu_1 \\ -\epsilon_1\mu_1 \end{bmatrix}.
\end{aligned} \tag{3.28}$$

- Third order jump condition: $\dfrac{1}{\epsilon_1\mu_1^2}E^{(3)}(t,\xi^-) = \dfrac{1}{\epsilon_2\mu_2^2}E^{(3)}(t,\xi^+)$. We have

$$
\begin{aligned}
&\frac{1}{\epsilon_1\mu_1^2}\left[\frac{-1}{2}g_{-2} + g_{-1} + 0g_0 - f_1 + \frac{1}{2}f_2\right] \\
&\qquad\qquad = \frac{1}{\epsilon_2\mu_2^2}\left[\frac{-1}{2}f_{-2} + f_{-1} + 0g_0 - g_1 + \frac{1}{2}g_2\right] \\
&\implies \frac{1}{\epsilon_2\mu_2^2}f_{-2} + \frac{-2}{\epsilon_2\mu_2^2}f_{-1} + \frac{-2}{\epsilon_1\mu_1^2}f_1 + \frac{1}{\epsilon_1\mu_1^2}f_2 \\
&\qquad\qquad = \frac{1}{\epsilon_1\mu_1^2}g_{-2} + \frac{-2}{\epsilon_1\mu_1^2}g_{-1} + 0 + \frac{-2}{\epsilon_2\mu_2^2}g_1 + \frac{1}{\epsilon_2\mu_2^2}g_2 \\
&\implies \epsilon_1\mu_1^2R_1^T - 2\epsilon_1\mu_1^2R_2^T - 2\epsilon_2\mu_2^2R_4^T + \epsilon_2\mu_2^2R_5^T = \begin{bmatrix} \epsilon_2\mu_2^2 \\ -2\epsilon_2\mu_2^2 \\ 0 \\ -2\epsilon_1\mu_1^2 \\ \epsilon_1\mu_1^2 \end{bmatrix}.
\end{aligned}
\tag{3.29}
$$

- Fourth order jump condition: $\dfrac{1}{\epsilon_1^2\mu_1^2}E^{(4)}(t,\xi^-) = \dfrac{1}{\epsilon_2^2\mu_2^2}E^{(4)}(t,\xi^+)$. We have

$$
\begin{aligned}
&\frac{1}{\epsilon_1^2\mu_1^2}\left[g_{-2} - 4g_{-1} + 6g_0 - 4f_1 + f_2\right] = \frac{1}{\epsilon_2^2\mu_2^2}\left[f_{-2} - 4f_{-1} + 6g_0 - 4g_1 + g_2\right] \\
&\implies \frac{-1}{\epsilon_2^2\mu_2^2}f_{-2} + \frac{4}{\epsilon_2^2\mu_2^2}f_{-1} + \frac{-6}{\epsilon_2^2\mu_2^2}f_0 + \frac{-4}{\epsilon_1^2\mu_1^2}f_1 + \frac{1}{\epsilon_1^2\mu_1^2}f_2 \\
&\qquad\qquad = \frac{-1}{\epsilon_1^2\mu_1^2}g_{-2} + \frac{4}{\epsilon_1^2\mu_1^2}g_{-1} + \frac{-6}{\epsilon_1^2\mu_1^2}g_0 + \frac{-4}{\epsilon_2^2\mu_2^2}g_1 + \frac{1}{\epsilon_2^2\mu_2^2}g_2 \\
&\implies -\epsilon_1^2\mu_1^2R_1^T + 4\epsilon_1^2\mu_1^2R_2^T - 6\epsilon_1^2\mu_1^2R_3^T - 4\epsilon_2^2\mu_2^2R_4^T + \epsilon_2^2\mu_2^2R_5^T = \begin{bmatrix} -\epsilon_2^2\mu_2^2 \\ 4\epsilon_2^2\mu_2^2 \\ -6\epsilon_2^2\mu_2^2 \\ -4\epsilon_1^2\mu_1^2 \\ 1\epsilon_1^2\mu_1^2 \end{bmatrix}.
\end{aligned}
\tag{3.30}
$$

Now put together the equations (3.26), (3.27), (3.28), (3.29), (3.30) to get following the system for R^E.

$$\begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ -\mu_1 & 8\mu_1 & 0 & 8\mu_2 & -\mu_2 \\ \epsilon_1\mu_1 & -16\epsilon_1\mu_1 & 30\epsilon_1\mu_1 & 16\epsilon_2\mu_2 & -\epsilon_2\mu_2 \\ \epsilon_1\mu_1^2 & -2\epsilon_1\mu_1^2 & 0 & -2\epsilon_2\mu_2^2 & \epsilon_2\mu_2^2 \\ -\epsilon_1^2\mu_1^2 & 4\epsilon_1^2\mu_1^2 & -6\epsilon_1^2\mu_1^2 & -4\epsilon_2^2\mu_2^2 & \epsilon_2^2\mu_2^2 \end{bmatrix} R^E$$

$$= \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ -\mu_2 & 8\mu_2 & 0 & 8\mu_1 & -\mu_1 \\ \epsilon_2\mu_2 & -16\epsilon_2\mu_2 & 30\epsilon_2\mu_2 & 16\epsilon_1\mu_1 & -\epsilon_1\mu_1 \\ \epsilon_2\mu_2^2 & -2\epsilon_2\mu_2^2 & 0 & -2\epsilon_1\mu_1^2 & \epsilon_1\mu_1^2 \\ -\epsilon_2^2\mu_2^2 & 4\epsilon_2^2\mu_2^2 & -6\epsilon_2^2\mu_2^2 & -4\epsilon_1^2\mu_1^2 & \epsilon_1^2\mu_1^2 \end{bmatrix}.$$

3.6.2 Numerical Experiment

Recall in Section 3.3. we had the exact solution (3.11) for Maxwell's equations in a dielectric medium with a material interface. We demonstrated that the accuracy of the (2,4) scheme was reduced to first order due to the presence of the material interface. Now we use the same initial conditions derived from (3.11) and apply the (2,4) scheme with IDM modification. Table 3.4 gives the results of this experiment and clearly we have the fourth order rate of convergence restored to the (2,4) scheme. Figure 3.9 shows the fourth order accuracy in a log-log plot.

TABLE 3.4: Error in L^2 norm for the (2,4) scheme with IDM modification in a dielectric with one interface. The spatial step size Δz and the Courant number $\nu = \frac{c\Delta t}{\Delta z}$ are reduced by half each time. Then the time step Δt is reduced by one fourth each time so that we can see the fourth order accuracy in space.

ν	Δz	**E** L^2 **error**	**ratio**	**rate**	**H** L^2 **error**	**ratio**	**rate**
0.8	0.04	0.034928	-	-	0.043867	-	-
0.4	0.02	0.0021825	16.003	4.0003	0.0027401	16.009	4.0008
0.2	0.01	0.00013631	16.012	4.0011	0.00017111	16.014	4.0013
0.1	0.005	8.5178e-06	16.002	4.0002	1.0692e-05	16.003	4.0003
0.05	0.0025	5.3239e-07	15.999	3.9999	6.6829e-07	15.999	3.9999
0.025	0.00125	3.3274e-08	16	4	4.1768e-08	16	4

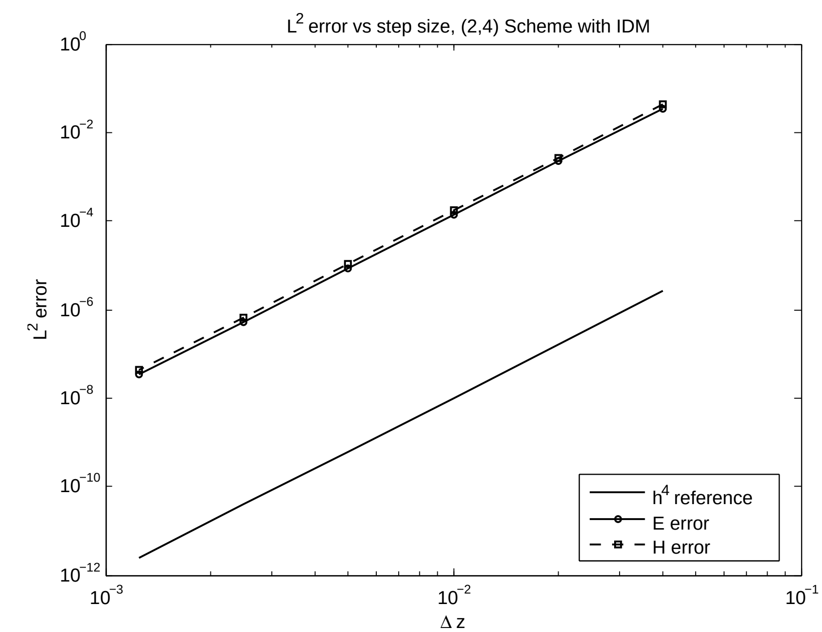


FIGURE 3.9: Log plots show the (2,4) scheme with the IDM modification is fourth order accurate in space.

4. IMPLICIT DERIVATIVE MATCHING TECHNIQUE FOR DISPERSIVE DIELECTRICS

4.1. Introduction

In this chapter we extend the IDM technique to modify the Yee scheme in dispersive media of Debye type. For this media we obtain jump conditions by requiring that the electric field E, the magnetic field H, and the polarization P, and their time derivatives are all continuous across an interface. Material interfaces represent discontinuities in the parameters of the medium, namely the infinite frequency permittivity ϵ_∞, the zero frequency permittivity ϵ_s, and the relaxation time τ. We place fictitious points for E, H, and P at appropriate locations in order to implement the jump conditions. For a scheme of spatial order $2m(m \geq 1)$ we need $2m$ fictitious points as in the IDM technique derived in Chapter 3 for dielectrics. However, for Debye media, we have to make a different assumption regarding the representation coefficients. We make the assumption that the electric field fictitious points are given as linear combinations of $2m$ actual electric field values. The polarization field fictitious points are given as linear combinations of $2m$ actual electric field values and $2m$ actual polarization field values. Finally, the magnetic field fictitious points are given as linear combinations of $2m$ actual electric field, polarization field and magnetic field values. This modification in the representation of the fictitious values for the three fields has to be made due to the presence of zero order terms in the partial differential equations for the three fields, and such an assumption avoids an overdetermined system for the fictitious values.

First we derive a scaled model of Maxwell's equations in Debye media in Section 4.2. We develop the IDM technique as outlined above for the Yee scheme in Debye media in Sections 4.3 and 4.4. In order to do this, we derive an exact solution for Maxwell's equations with Debye polarization using reflection-transmission analysis in Section 4.5.

In Section 4.6, we demonstrate the loss of accuracy to first order for a problem with a material interface using the Yee scheme without modification. In addition, we modify the Yee scheme locally around material interfaces using the IDM technique and demonstrate second order accuracy for the same interface problem. We conclude with a discussion of the extension of the IDM technique for the modification of $2m(m > 1)$ order in space FDTD schemes to maintain $2m$ order spatial accuracy.

4.2. Model Formulation

Recall Maxwell's equations plus Debye polarization in one dimension are

$$\frac{\partial H}{\partial t} = \frac{1}{\mu_0}\frac{\partial E}{\partial z} \tag{4.1a}$$

$$\epsilon_0\epsilon_\infty\frac{\partial E}{\partial t} = \frac{\partial H}{\partial z} - \frac{\epsilon_0\epsilon_d}{\tau}E + \frac{1}{\tau}P \tag{4.1b}$$

$$\frac{\partial P}{\partial t} = \frac{\epsilon_0\epsilon_d}{\tau}E - \frac{1}{\tau}P, \tag{4.1c}$$

where $\epsilon_d = \epsilon_s - \epsilon_\infty$. We will re-scale the equations in order to simplify calculations in the forthcoming sections. To do this, we assume the following relations:

$$\begin{aligned} &\tilde{E} = \sqrt{\epsilon_0}E, \quad \tilde{P} = \frac{1}{\sqrt{\epsilon_0}}P, \quad \tilde{H} = \sqrt{\mu_0}H, \\ &\tilde{t} = \frac{t}{\tau}, \quad \tilde{z} = \frac{z}{c_0\tau}, \end{aligned} \tag{4.2}$$

where c_0 is the speed of light. Note that from the relations (4.2) we get

$$\begin{aligned} \frac{\partial}{\partial t} &= \frac{\partial}{\partial \tilde{t}}\frac{\partial \tilde{t}}{t} = \frac{1}{\tau}\frac{\partial}{\partial \tilde{t}}, \\ \frac{\partial}{\partial z} &= \frac{\partial}{\partial \tilde{z}}\frac{\partial \tilde{z}}{z} = \frac{1}{c_0\tau}\frac{\partial}{\partial \tilde{z}}. \end{aligned}$$

Now we use the scalings to transform the system (4.1), starting with the equation for $\dfrac{\partial H}{\partial t}$.

$$\begin{aligned} \frac{\partial H}{\partial t} &= \frac{1}{\mu_0}\frac{\partial E}{\partial z} \\ \Longrightarrow \quad \frac{1}{\sqrt{\mu_0}}\frac{\partial \tilde{H}}{\partial t} &= \frac{1}{\mu_0\sqrt{\epsilon_0}}\frac{\partial \tilde{E}}{\partial z} \end{aligned}$$

$$\begin{aligned}
\implies \frac{\partial \tilde{H}}{\partial t} &= \frac{1}{\sqrt{\mu_0}\sqrt{\epsilon_0}}\frac{\partial \tilde{E}}{\partial z} = c_0\frac{\partial \tilde{E}}{\partial z} \\
\implies \frac{1}{\tau}\frac{\partial \tilde{H}}{\partial \tilde{t}} &= \frac{1}{c_0\tau}c_0\frac{\partial \tilde{E}}{\partial \tilde{z}} \\
\implies \frac{\partial \tilde{H}}{\partial \tilde{t}} &= \frac{\partial \tilde{E}}{\partial \tilde{z}} \qquad (4.3)
\end{aligned}$$

Next we scale the equation for $\dfrac{\partial E}{\partial t}$.

$$\begin{aligned}
\epsilon_0\epsilon_\infty\frac{\partial E}{\partial t} &= \frac{\partial H}{\partial z} - \frac{\epsilon_0\epsilon_d}{\tau}E + \frac{1}{\tau}P \\
\implies \sqrt{\epsilon_0}\epsilon_\infty\frac{\partial \tilde{E}}{\partial t} &= \frac{1}{\sqrt{\mu_0}}\frac{\partial \tilde{H}}{\partial z} - \frac{\sqrt{\epsilon_0}\epsilon_d}{\tau}\tilde{E} + \frac{\sqrt{\epsilon_0}}{\tau}\tilde{P} \\
\implies \frac{\epsilon_\infty}{\tau}\frac{\partial \tilde{E}}{\partial \tilde{t}} &= \frac{c_0}{c_0\tau}\frac{\partial \tilde{H}}{\partial \tilde{z}} - \frac{\epsilon_d}{\tau}\tilde{E} + \frac{1}{\tau}\tilde{P} \\
\implies \epsilon_\infty\frac{\partial \tilde{E}}{\partial \tilde{t}} &= \frac{\partial \tilde{H}}{\partial \tilde{z}} - \epsilon_d\tilde{E} + \tilde{P} \qquad (4.4)
\end{aligned}$$

And finally we scale the equation for $\dfrac{\partial P}{\partial t}$.

$$\begin{aligned}
\frac{\partial P}{\partial t} &= \frac{\epsilon_0\epsilon_d}{\tau}E - \frac{1}{\tau}P \\
\implies \frac{\sqrt{\epsilon_0}}{\tau}\frac{\partial \tilde{P}}{\partial \tilde{t}} &= \frac{\sqrt{\epsilon_0}\epsilon_d}{\tau}\tilde{E} - \frac{\sqrt{\epsilon_0}}{\tau}\tilde{P} \\
\implies \frac{\partial \tilde{P}}{\partial \tilde{t}} &= \epsilon_d\tilde{E} - \tilde{P} = \epsilon_\infty(\epsilon_q - 1)\tilde{E} - \tilde{P}, \qquad (4.5)
\end{aligned}$$

where $\epsilon_q = \epsilon_s/\epsilon_\infty$. The new scaled system for Debye media (drop the $\sim$ to simplify notation) is

$$\begin{aligned}
\frac{\partial H}{\partial t} &= \frac{\partial E}{\partial z}, \\
\frac{\partial E}{\partial t} &= \frac{1}{\epsilon_\infty}\frac{\partial H}{\partial z} - (\epsilon_q - 1)E + \frac{1}{\epsilon_\infty}P, \qquad (4.6) \\
\frac{\partial P}{\partial t} &= \epsilon_\infty(\epsilon_q - 1)E - P.
\end{aligned}$$

Note that in this scaled version $\epsilon_0 = \mu_0 = \tau = 1$. We can write our system as a matrix equation as in Section 3.4.

$$\frac{\partial \mathbf{u}}{\partial t} = A\frac{\partial \mathbf{u}}{\partial z} + B\mathbf{u}, \qquad (4.7)$$

$$\text{with } \mathbf{u} = \begin{bmatrix} E \\ P \\ H \end{bmatrix}, \; A = \begin{bmatrix} 0 & 0 & \dfrac{1}{\epsilon_\infty} \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \text{ and } B = \begin{bmatrix} -(\epsilon_q - 1) & \dfrac{1}{\epsilon_\infty} & 0 \\ \epsilon_\infty(\epsilon_q - 1) & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

In a heterogeneous material, we will have A_1 in medium 1 and A_2 in medium 2, and similarly for B, i.e.,

$$A_i = \begin{bmatrix} 0 & 0 & \dfrac{1}{\epsilon_{\infty,i}} \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix} \text{ and } B_i = \begin{bmatrix} -(\epsilon_{q,i} - 1) & \dfrac{1}{\epsilon_{\infty,i}} & 0 \\ \epsilon_{\infty,i}(\epsilon_{q,i} - 1) & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}. \tag{4.8}$$

4.3. Derivation of Jump Conditions

As before, we impose the following interface conditions

$$\mathbf{n} \times (\mathbf{E}_1 - \mathbf{E}_2) = \mathbf{0}, \qquad \mathbf{n} \cdot (\mathbf{D}_1 - \mathbf{D}_2) = 0,$$

$$\mathbf{n} \times (\mathbf{H}_1 - \mathbf{H}_2) = \mathbf{0}, \qquad \mathbf{n} \cdot (\mathbf{B}_1 - \mathbf{B}_2) = 0,$$

where $\mathbf{D} = \epsilon_0 \epsilon_\infty \mathbf{E} + \mathbf{P}$ and $\mathbf{B} = \mu_0 \mathbf{H}$, and $\mathbf{n}$ is the unit normal vector to the interface. Additionally, for the polarization P we assume that

$$P_1 = P(t, \xi^-), \; P_2 = P(t, \xi^+), \text{ where } \mathbf{P_i} = (0, P_i, 0), \; i = 1, 2,$$

$$\text{and } \mathbf{n} \times (\mathbf{P}_1 - \mathbf{P}_2) = \mathbf{0} \implies P_1 - P_2.$$

The zeroth order jump conditions can be derived from the interface conditions, as for the dielectric case in Section 3.4.

$$\mathbf{u}^{(0)}(t, \xi^-) = \mathbf{u}^{(0)}(t, \xi^+).$$

As before, we assume that the time derivatives are also continuous, so we have

$$\frac{\partial \mathbf{u}^{(0)}}{\partial t}(t, \xi^-) = \frac{\partial \mathbf{u}^{(0)}}{\partial t}(t, \xi^+).$$

The differential equation (4.7) then gives us

$$A_1\mathbf{u}^{(1)}(t,\xi^-) + B_1\mathbf{u}^{(0)}(t,\xi^-) = A_2\mathbf{u}^{(1)}(t,\xi^+) + B_2\mathbf{u}^{(0)}(t,\xi^+), \tag{4.9}$$

where A_i, B_i are the coefficient matrices for media $i = 1,2$ (see Equation (4.8)). Clearly, on either side of the interface the time derivative $\dfrac{\partial}{\partial t}$ is equivalent to $A_i\dfrac{\partial}{\partial z} + B_i$. We can apply the time derivative as many times as we like in order to get any pth order jump condition. For example, we will derive the second order jump condition from (4.9).

$$\begin{aligned}
&\frac{\partial}{\partial t}\left(A_1\mathbf{u}^{(1)}(t,\xi^-) + B_1\mathbf{u}^{(0)}(t,\xi^-)\right) = \frac{\partial}{\partial t}\left(A_2\mathbf{u}^{(1)}(t,\xi^+) + B_2\mathbf{u}^{(0)}(t,\xi^+)\right)\\
&\implies \left(A_1\frac{\partial}{\partial z} + B_1\right)\left(A_1\mathbf{u}^{(1)}(t,\xi^-) + B_1\mathbf{u}^{(0)}(t,\xi^-)\right)\\
&\qquad\qquad = \left(A_2\frac{\partial}{\partial z} + B_2\right)\left(A_2\mathbf{u}^{(1)}(t,\xi^+) + B_2\mathbf{u}^{(0)}(t,\xi^+)\right)\\
&\implies A_1^2\mathbf{u}^{(2)}(t,\xi^-) + A_1B_1\mathbf{u}^{(1)}(t,\xi^-) + B_1A_1\mathbf{u}^{(1)}(t,\xi^-) + B_1^2\mathbf{u}^{(0)}(t,\xi^-)\\
&\qquad\qquad = A_2^2\mathbf{u}^{(2)}(t,\xi^+) + A_2B_2\mathbf{u}^{(1)}(t,\xi^+) + B_2A_2\mathbf{u}^{(1)}(t,\xi^+) + B_2^2\mathbf{u}^{(0)}(t,\xi^+).
\end{aligned}$$

In general, we can write the pth order jump condition as

$$\left(A_1\frac{\partial}{\partial z} + B_1\right)^p \mathbf{u}^{(0)}(t,\xi^-) = \left(A_2\frac{\partial}{\partial z} + B_2\right)^p \mathbf{u}^{(0)}(t,\xi^+).$$

4.4. IDM for Yee Scheme in Debye Media

The implicit derivative matching technique for the Yee scheme ($m = 1$) in dielectric materials required $2m = 2$ fictitious points for both E and H, so there are 4 fictitious points total. Now we have three fields to consider, E, P, H, so we have $3 \times 2m = 6m = 6$ fictitious points in total. Unlike the dielectric case, the jump conditions do not decouple for Debye media. This means we will have only one 6×6 matrix of representation coefficients. As before, we use up to the $(2m-1)$th order jump conditions to construct the system to solve for R, so we only need the zeroth and first order conditions for the Yee scheme.

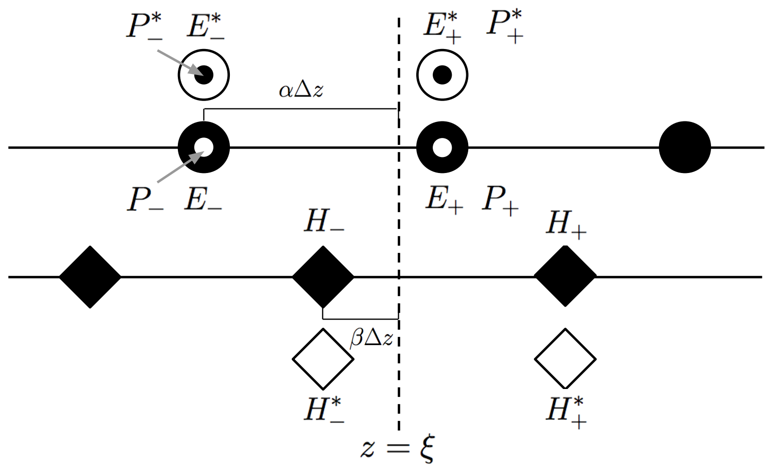


FIGURE 4.1: Fictitious points needed in the IDM modification of the Yee scheme are designated by *. In general, the distance of E_- from the interface is $\alpha\Delta z$ and $\beta\Delta z$ is the distance for H_-, where $\alpha, \beta \in [0, \frac{1}{2}]$ and $|\alpha - \beta| = \frac{1}{2}$. α and β are used to calculate the weights for discretizing the derivative jump conditions.

Let $G = [E_-,\, E_+,\, P_-,\, P_+,\, H_-,\, H_+]^T$, where Figure 4.1 shows the positions of the needed nodes. The new assumptions for the representation of the fictitious points are

$$
\begin{aligned}
E_i^* &= \sum_{j=1}^{2m} r_{ij}^{E} E_j, \\
P_i^* &= \sum_{j=1}^{2m} r_{ij}^{PE} E_j + \sum_{j=1}^{2m} r_{ij}^{P} P_j, \\
H_i^* &= \sum_{j=1}^{2m} r_{ij}^{HE} E_j + \sum_{j=1}^{2m} r_{ij}^{HP} P_j + \sum_{j=1}^{2m} r_{ij}^{H} H_j.
\end{aligned}
$$

In this case the structure of the representation matrix R is

$$
R = \begin{bmatrix} R^E & & \\ R^{PE} & R^P & \\ R^{HE} & R^{HP} & R^H \end{bmatrix},
$$

where each R^V is a 2×2 block. Then we have the following definitions for the fictitious points, where R_i is the ith row of R.

$$
E_-^* = R_1 G, \qquad E_+^* = R_2 G,
$$

$$P_-^* = R_3 G, \qquad P_+^* = R_4 G,$$

$$H_-^* = R_5 G, \qquad H_+^* = R_6 G.$$

Now we are ready to discretize the zeroth and first order jump conditions that we derived in Section 4.3. The zeroth order jump conditions are straightforward to discretize, because they are the same as for the Yee scheme in dielectrics, with the addition of the P equation. With the positioning of the nodes in Figure 4.1, the zeroth derivative weights for E and P are $\{1-\alpha, \alpha\}$, and the weights for H are $\{1-\beta, \beta\}$.

$$\begin{aligned}
& E^{(0)}(t, \xi^-) = E^{(0)}(t, \xi^+) \\
\implies & (1-\alpha)E_- + \alpha E_+^* = (1-\alpha)E_-^* + \alpha E_+ \\
\implies & -(1-\alpha)E_-^* + \alpha E_+^* = -(1-\alpha)E_- + \alpha E_+ \\
\implies & -(1-\alpha)R_1 G + \alpha R_2 G = -(1-\alpha)I_1 G + \alpha I_2 G \\
\implies & -(1-\alpha)R_1 + \alpha R_2 = \begin{bmatrix} -(1-\alpha), & \alpha \end{bmatrix}.
\end{aligned} \tag{4.10}$$

We do the same discretization for P and H conditions to get:

$$\begin{aligned}
& P^{(0)}(t, \xi^-) = P^{(0)}(t, \xi^+) \\
\implies & -(1-\alpha)R_3 + \alpha R_4 = \begin{bmatrix} -(1-\alpha), & \alpha \end{bmatrix},
\end{aligned} \tag{4.11}$$

$$\begin{aligned}
& H^{(0)}(t, \xi^-) = H^{(0)}(t, \xi^+) \\
\implies & -(1-\beta)R_5 + \beta R_6 = \begin{bmatrix} -(1-\beta), & \beta \end{bmatrix}.
\end{aligned} \tag{4.12}$$

The weights for discretizing the first derivative are $\{-1/\Delta z,\ 1/\Delta z\}$ for all three fields. Note that for $\alpha = 0$, and $\beta = 1/2$, i.e., the case where the nodes are symmetrically placed around the interface, the first derivative discretization is second order accurate. However, in all of the other cases where the nodes are not symmetric around the interface, this discretization is only first order accurate. In our experiments, we will consider the symmetric case, but note that the IDM will need to be modified in the asymmetric case so that we maintain second order accuracy of the IDM-Yee scheme. Of course, we can always choose our grid so that the nodes are symmetric about the interface, and then the above method will give second order accuracy.

Now we discretize the first order jump conditions. We start with the first order jump condition on H.

$$\begin{aligned}
&\frac{1}{\epsilon_{\infty,1}}H^{(1)}(t,\xi^-) + \frac{1}{\epsilon_{\infty,1}}P^{(0)}(t,\xi^-) - (\epsilon_{q,1}-1)E^{(0)}(t,\xi^-) \\
&\quad = \frac{1}{\epsilon_{\infty,2}}H^{(1)}(t,\xi^+) + \frac{1}{\epsilon_{\infty,2}}P^{(0)}(t,\xi^+) - (\epsilon_{q,2}-1)E^{(0)}(t,\xi^+) \\
&\Rightarrow \frac{1}{\epsilon_{\infty,1}\Delta z}(-H_{-1/2} + H^*_{1/2}) + \frac{1}{\epsilon_{\infty,1}}((1-\alpha)P_{-1} + \alpha P^*_1) - (\epsilon_{q,1}-1)((1-\alpha)E_{-1} + \alpha E^*_1) \\
&\quad = \frac{1}{\epsilon_{\infty,2}\Delta z}(-H^*_{-1/2} + H_{1/2}) + \frac{1}{\epsilon_{\infty,2}}((1-\alpha)P^*_{-1} + \alpha P_1) - (\epsilon_{q,2}-1)((1-\alpha)E^*_{-1} + \alpha E_1) \\
&\Rightarrow \frac{1}{\epsilon_{\infty,2}\Delta z}R_5 + \frac{1}{\epsilon_{\infty,1}\Delta z}R_6 - \frac{1-\alpha}{\epsilon_{\infty,2}}R_3 + \frac{\alpha}{2\epsilon_{\infty,1}}R_4 + (\epsilon_{q,2}-1)(1-\alpha)R_1 - (\epsilon_{q,1}-1)\alpha R_2 \\
&\quad = \left[\frac{1}{\epsilon_{\infty,1}\Delta z},\quad \frac{1}{\epsilon_{\infty,2}\Delta z},\quad -\frac{1-\alpha}{\epsilon_{\infty,1}},\quad \frac{\alpha}{\epsilon_{\infty,2}},\quad (1-\alpha)(\epsilon_{q,1}-1),\quad -\alpha(\epsilon_{q,2}-1)\right]. \qquad (4.13)
\end{aligned}$$

It is important to note that we have not said anything about the time step. In the dielectric case, each jump condition only involved one of the fields, so everything was at the same time step. Now we have a condition that involves all three fields, and we only know H at half time steps and E, P at full time steps. We actually have E^n_-, E^n_+ and $H^{n+1/2}_-$, $H^{n+1/2}_+$, but have dropped the time step information to simplify notation. Now we discretize the first order condition for E.

$$\begin{aligned}
E^{(1)}(t,\xi^-) &= E^{(1)}(t,\xi^+) \\
\Longrightarrow\ -\frac{1}{\Delta z}E_- + \frac{1}{\Delta z}E^*_+ &= -\frac{1}{\Delta z}E^*_- + \frac{1}{\Delta z}E_+ \\
\Longrightarrow\ E^*_- + E^*_+ &= E_- + E_+ \\
\Longrightarrow\ R_1G + R_2G &= I_1G + I_2G \\
\Longrightarrow\ R_1 + R_2 &= \begin{bmatrix}1, & 1\end{bmatrix}. \qquad (4.14)
\end{aligned}$$

Finally we discretize the first order jump condition for P.

$$\begin{aligned}
&\epsilon_{d,1}E^{(0)}(t,\xi^-) - P^{(0)}(t,\xi^-) = \epsilon_{d,2}E^{(0)}(t,\xi^+) - P^{(0)}(t,\xi^+) \\
\implies &\epsilon_{d,1}((1-\alpha)E_- + \alpha E_+^*) - ((1-\alpha)P_- + \alpha P_+^*) \\
&\qquad = \epsilon_{d,2}((1-\alpha)E_-^* + \alpha E_+) - ((1-\alpha)P_-^* + \alpha P_+) \\
\implies &-\epsilon_{d,2}(1-\alpha)E_-^* + \epsilon_{d,1}\alpha E_+^* + (1-\alpha)P_-^* - \alpha P_+^* \\
&\qquad = -\epsilon_{d,1}(1-\alpha)E_- + \epsilon_{d,2}\alpha E_+ + (1-\alpha)P_- - \alpha P_+ \\
\implies &-(1-\alpha)\epsilon_{d,2}R_1 + \alpha\epsilon_{d,1}R_2 + (1-\alpha)R_3 - \alpha R_4 \\
&\qquad = \begin{bmatrix} -(1-\alpha)\epsilon_{d,1}, & \alpha\epsilon_{d,2}, & (1-\alpha), & -\alpha \end{bmatrix}.
\end{aligned} \tag{4.15}$$

Now we can put together the equations (4.10) through (4.15), and solve the system $CR = D$ using LU factorization with partial pivoting (via MATLAB's `linsolve` function), where

$$C = \begin{bmatrix}
-(1-\alpha) & \alpha & 0 & 0 & 0 & 0 \\
\frac{1}{\Delta z} & \frac{1}{\Delta z} & 0 & 0 & 0 & 0 \\
0 & 0 & -(1-\alpha) & \alpha & 0 & 0 \\
-(1-\alpha)\epsilon_{d,2} & \alpha\epsilon_{d,1} & (1-\alpha) & -\alpha & 0 & 0 \\
0 & 0 & 0 & 0 & -(1-\beta) & \beta \\
(1-\alpha)(\epsilon_{q,2}-1) & -\alpha(\epsilon_{q,1}-1) & \frac{-(1-\alpha)}{\epsilon_{\infty,2}} & \frac{\alpha}{\epsilon_{\infty,1}} & \frac{1}{\Delta z\epsilon_{\infty,2}} & \frac{1}{\Delta z\epsilon_{\infty,1}},
\end{bmatrix}$$

$$D = \begin{bmatrix}
-(1-\alpha) & \alpha & 0 & 0 & 0 & 0 \\
\frac{1}{\Delta z} & \frac{1}{\Delta z} & 0 & 0 & 0 & 0 \\
0 & 0 & -(1-\alpha) & \alpha & 0 & 0 \\
-(1-\alpha)\epsilon_{d,1} & \alpha\epsilon_{d,2} & (1-\alpha) & -\alpha & 0 & 0 \\
0 & 0 & 0 & 0 & -(1-\beta) & \beta \\
(1-\alpha)(\epsilon_{q,1}-1) & -\alpha(\epsilon_{q,2}-1) & \frac{-(1-\alpha)}{\epsilon_{\infty,1}} & \frac{\alpha}{\epsilon_{\infty,2}} & \frac{1}{\Delta z\epsilon_{\infty,1}} & \frac{1}{\Delta z\epsilon_{\infty,2}}
\end{bmatrix}.$$

Once the representation coefficients are obtained, we can modify the Yee scheme for Debye media, given in (2.36), around the interface.

4.5. Reflection-Transmission Analysis

Before using the IDM to modify the Yee scheme in a heterogeneous Debye medium, an exact solution is needed. We use reflection-transmission analysis to develop the exact solution as in Section 3.2. We assume the following forms for E and H in the domain $\Omega = [-1, 1]$.

$$E(t,z) = \begin{cases} \omega E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + \omega E_1^- \mathrm{e}^{i(\omega t + k_1 z)}, & -1 \le z \le 0 \\ \omega E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + \omega E_2^- \mathrm{e}^{i(\omega t + k_2 z)}, & 0 \le z \le 1 \end{cases} \tag{4.16}$$

$$H(t,z) = \begin{cases} H_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + H_1^- \mathrm{e}^{i(\omega t + k_1 z)}, & -1 \le z \le 0 \\ H_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + H_2^- \mathrm{e}^{i(\omega t + k_2 z)}, & 0 \le z \le 1 \end{cases} \tag{4.17}$$

Note that $E_j^\pm$ and $H_j^\pm$ are coefficients that we need to determine, k_j is the wave number for media j, and ω is the angular frequency. From Maxwell's equations, we have $\dfrac{\partial H}{\partial t} = \dfrac{\partial E}{\partial z}$ (4.1a) and with the above forms for E, H it is easy to see

$$\begin{aligned} i\omega H_1^+ &= (-ik_1)\omega E_1^+ \implies H_1^+ = -k_1 E_1^+, \\ i\omega H_1^- &= (ik_1)\omega E_1^- \implies H_1^- = k_1 E_1^-, \\ i\omega H_2^+ &= (-ik_2)\omega E_2^+ \implies H_2^+ = -k_2 E_2^+, \\ i\omega H_2^- &= (ik_2)\omega E_2^- \implies H_2^- = k_2 E_2^-. \end{aligned}$$

Then we can rewrite the H representation (4.17) as

$$H(t,z) = \begin{cases} -k_1 E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + k_1 E_1^- \mathrm{e}^{i(\omega t + k_1 z)}, & -1 \le z \le 0 \\ -k_2 E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + k_2 E_2^- \mathrm{e}^{i(\omega t + k_2 z)}, & 0 \le z \le 1 \end{cases} \tag{4.18}$$

Now we need to find a form for P by substituting (4.16) and (4.18) into the equation (4.1b) from Maxwell's equations. This implies that

$$\begin{aligned}\frac{\partial P}{\partial t}(t,z) &= \left(ik_1^2 E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + ik_1^2 E_1^- \mathrm{e}^{i(\omega t + k_1 z)}\right)\chi_{[-1,0]} \\ &\quad + \left(ik_2^2 E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + ik_2^2 E_2^- \mathrm{e}^{i(\omega t + k_2 z)}\right)\chi_{[0,1]} \\ &\quad - \epsilon_{\infty,1}\left(i\omega^2 E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + i\omega^2 E_1^- \mathrm{e}^{i(\omega t + k_1 z)}\right)\chi_{[-1,0]} \\ &\quad - \epsilon_{\infty,2}\left(i\omega^2 E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + i\omega^2 E_2^- \mathrm{e}^{i(\omega t + k_2 z)}\right)\chi_{[0,1]}.\end{aligned}$$

Thus,

$$\begin{aligned}\frac{\partial P}{\partial t}(t,z) &= i(k_1^2 - \epsilon_{\infty,1}\omega^2)\left(E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + E_1^- \mathrm{e}^{i(\omega t + k_1 z)}\right)\chi_{[-1,0]} \\ &\quad + i(k_2^2 - \epsilon_{\infty,2}\omega^2)\left(E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + E_2^- \mathrm{e}^{i(\omega t + k_2 z)}\right)\chi_{[0,1]},\end{aligned} \tag{4.19}$$

where $\chi_{[a,b]}$ is the characteristic function on the interval $[a,b]$. Now we can substitute (4.19) along with (4.16) into (4.1c) from Maxwell's equations to find P, as

$$\begin{aligned}P(t,z) &= \epsilon_{d,1}\left(\omega E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + \omega E_1^- \mathrm{e}^{i(\omega t + k_1 z)}\right)\chi_{[-1,0]} \\ &\quad + \epsilon_{d,2}\left(\omega E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + \omega E_2^- \mathrm{e}^{i(\omega t + k_2 z)}\right)\chi_{[-1,0]} \\ &\quad - i(k_1^2 - \epsilon_{\infty,1}\omega^2)\left(E_1^+ \mathrm{e}^{i(\omega t - k_1 z)} + E_1^- \mathrm{e}^{i(\omega t + k_1 z)}\right)\chi_{[-1,0]} \\ &\quad - i(k_2^2 - \epsilon_{\infty,2}\omega^2)\left(E_2^+ \mathrm{e}^{i(\omega t - k_2 z)} + E_2^- \mathrm{e}^{i(\omega t + k_2 z)}\right)\chi_{[0,1]}.\end{aligned}$$

Thus, we have the representation for P

$$P(t,z) = \begin{cases}(\epsilon_{d,1}\omega - ik_1^2 + i\epsilon_1\omega^2)[E_1^+ \mathrm{e}^{-ik_1 z)} + E_1^- \mathrm{e}^{ik_1 z)}]\mathrm{e}^{i\omega t},\ -1 \le z \le 0 \\ (\epsilon_{d,1}\omega - ik_1^2 + i\epsilon_1\omega^2)[E_2^+ \mathrm{e}^{-ik_2 z)} + E_2^- \mathrm{e}^{ik_2 z)}]\mathrm{e}^{i\omega t},\ 0 \le z \le 1\end{cases}. \tag{4.20}$$

Next we need to find the coefficients $E_1^+, E_1^-, E_2^+, E_2^-$. There are four constraints that our equations need to satisfy; continuity of E and H across the interface, and $E = 0$ on the boundaries. Applying the PEC boundary conditions to (4.16) gives us the following:

$$E_1^+ \mathrm{e}^{ik_1} + E_1^- \mathrm{e}^{-ik_1} = 0 \implies E_1^+ = -E_1^- \mathrm{e}^{-2ik_1}, \tag{4.21}$$

$$E_2^+ \mathrm{e}^{-ik_2} + E_2^- \mathrm{e}^{ik_2} = 0 \implies E_2^+ = -E_2^- \mathrm{e}^{2ik_2}. \tag{4.22}$$

Continuity at the interface gives us two more conditions on our coefficients

$$-k_1 E_1^+ + k_1 E_1^- = -k_2 E_2^+ + k_2 E_2^-, \tag{4.23}$$

$$E_1^+ + E_1^- = E_2^+ + E_2^-. \tag{4.24}$$

Now applying (4.21) and (4.22) to the continuity relations (4.23), (4.24) gives

$$E_1^- = E_2^- \frac{k_2(1+\mathrm{e}^{2ik_2})}{k_1(1+\mathrm{e}^{-2ik_1})}, \tag{4.25}$$

$$E_1^- = E_2^- \frac{1-\mathrm{e}^{2ik_2}}{1-\mathrm{e}^{-2ik_1}}. \tag{4.26}$$

We need a way to calculate the angular frequency ω, which is not straightforward as in homogeneous media. The dispersion relation for Debye media with normalized $\tau = 1$ is [3]

$$k = \frac{\omega}{c_\infty}\sqrt{\frac{\epsilon_q + i\omega}{1+i\omega}},$$

where $c_\infty = \dfrac{c_0}{\sqrt{\epsilon_\infty}}$. In a heterogeneous Debye medium, we have two wave numbers k_1, k_2 and one angular frequency ω that needs to satisfy the corresponding dispersion relations. We can relate k_1 to k_2 through (4.25) and (4.26). Then we have

$$\begin{aligned}
\frac{1-\mathrm{e}^{2ik_2}}{1-\mathrm{e}^{-2ik_1}} &= \frac{k_2(1+\mathrm{e}^{2ik_2})}{k_1(1+\mathrm{e}^{-2ik_1})} \\
\implies k_2\frac{1+\mathrm{e}^{2ik_2}}{1-\mathrm{e}^{2ik_2}} &= k_1\frac{1+\mathrm{e}^{-2ik_1}}{1-\mathrm{e}^{-2ik_1}} \\
\implies k_2\frac{-\cos(k_2)}{\sin(k_2)} &= k_1\frac{\cos(k_1)}{\sin(k_1)} \\
\implies -k_1\tan(k_2) &= k_2\tan(k_1).
\end{aligned} \tag{4.27}$$

The angular frequency ω can be found numerically from (4.27) if we substitute in the dispersion relations for k_1 and k_2, which gives us

$$-\frac{\omega}{c_{\infty,1}}\sqrt{\frac{\epsilon_{q,1}+i\omega}{1+i\omega}}\tan\left(\frac{\omega}{c_{\infty,2}}\sqrt{\frac{\epsilon_{q,2}+i\omega}{1+i\omega}}\right) = \frac{\omega}{c_{\infty,2}}\sqrt{\frac{\epsilon_{q,2}+i\omega}{1+i\omega}}\tan\left(\frac{\omega}{c_{\infty,1}}\sqrt{\frac{\epsilon_{q,1}+i\omega}{1+i\omega}}\right). \tag{4.28}$$

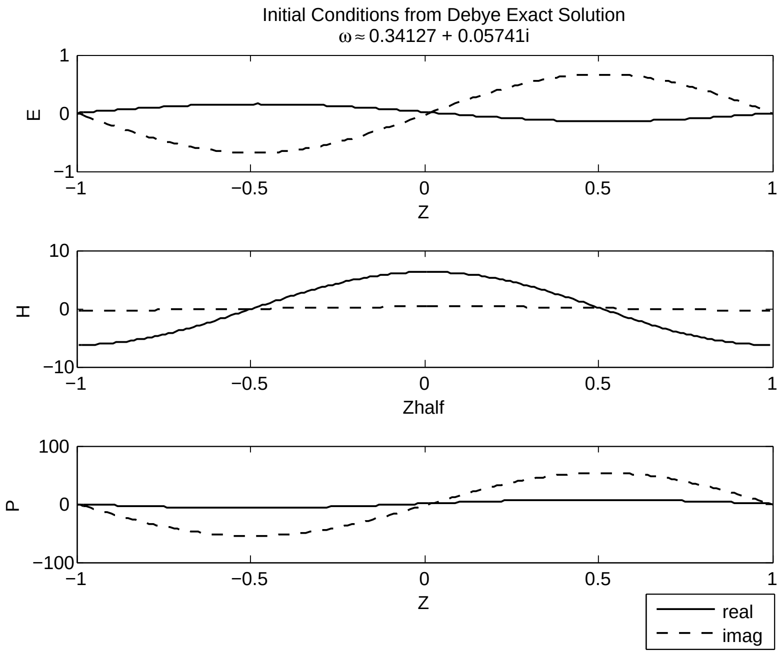


FIGURE 4.2: Initial conditions for Debye media given by the exact solution at time $t = 0$. Interface at $z = 0$.

There is one free parameter in the set of coefficients E_1^-, E_1^+, E_2^-, E_2^+. We choose $E_2^- = \mathrm{e}^{-i(k_1+k_2)}$ to be our free parameter. Applying this to (4.25) gives E_1^-, and subsequently, we can find E_1^+ and E_2^+ from (4.21), (4.22), respectively. Then our coefficients are

$$E_1^+ = -\frac{k_2 \cos(k_2)}{k_1 \cos(k_1)} \mathrm{e}^{-2ik_1}, \qquad E_1^- = \frac{k_2 \cos(k_2)}{k_1 \cos(k_1)},$$
$$E_2^+ = -\mathrm{e}^{-ik_1} \mathrm{e}^{ik_2}, \qquad E_2^- = \mathrm{e}^{-i(k_1+k_2)}.$$

4.6. Numerical Experiment

Figure 4.2 shows the initial conditions given by our exact solution at time $t = 0$. The following parameters were used to test the Yee scheme with and without the IDM modification.

$$z \in [-1,1] \text{ with interface at } z=0, \qquad t \in [0,\pi], \qquad \frac{c_\infty \Delta t}{\Delta z} = 1.0,$$

$$\epsilon_{s,1} = 80.35, \qquad \epsilon_{s,2} = 85.35, \qquad \epsilon_{\infty,1} = 1.0, \qquad \epsilon_{\infty,2} = 6.0,$$

$$k_1 \approx 3.09714 - 0.01514i, \qquad k_2 = 3.18718 + 0.01603i,$$

$$\omega \approx 0.34127 + 0.05741i.$$

The angular frequency ω was calculated numerically using MATLAB's `fsolve` function from the equation (4.28). The positioning of the interface requires that an electric field node be exactly on the interface, and hence also a polarization node. Thus, we have $\alpha = 0$ and $\beta = \frac{1}{2}$ in the setup of Figure 4.1.

Figure 4.3 shows that the solution is converging with first order accuracy for the Yee scheme without the IDM modification and the accuracy is restored when the IDM is applied. Note the absolute error uses the energy norm defined in Theorem 2.1.3.1.

$$\max_{0 \le t \le N\Delta t} \left[(\Delta z) \left(\epsilon_0 \epsilon_\infty \left\| E_{\text{num}} - E_{\text{ex}} \right\|_2^2 + \mu_0 \left\| H_{\text{num}} - H_{\text{ex}} \right\|_2^2 + \frac{1}{\epsilon_0 \epsilon_d} \left\| P_{\text{num}} - P_{\text{ex}} \right\|_2^2 \right) \right]^{1/2},$$

where V_{num} is the numerical solution and V_{ex} is the exact solution. Figure 4.4 shows the exact solution at the final time $t = \pi$. The scheme was also tested over a longer time period $t \in [0, 50\pi]$ and the time trace of this simulation is shown in Figure 4.5, which shows the numerical solution dissipates over the long period. Table 4.1 shows the Yee scheme in heterogeneous Debye media is first order accurate, while we see in Table 4.2 that the Yee scheme with IDM modification has second order accuracy.

4.7. Conclusion

The IDM technique developed in this chapter was successfully implemented in Debye media on a test problem for which an exact solution exists. Based on the results obtained in this chapter we now discuss the extension of the technique to higher order schemes. For

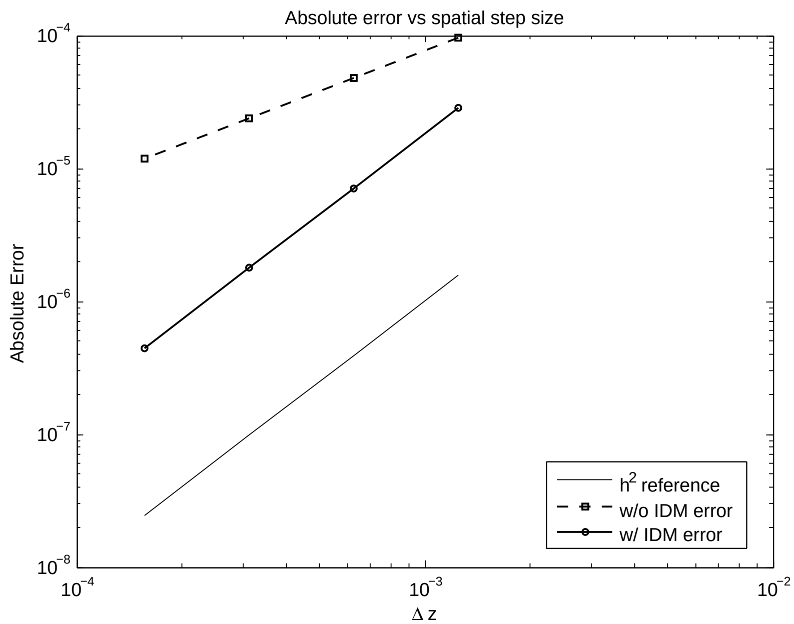


FIGURE 4.3: Log plot showing the Yee scheme is first order accurate without IDM modification (dashed line), while the Yee scheme with IDM modification is second order accurate (solid line with circles).

TABLE 4.1: Absolute error and rates of convergence without IDM modification.

Δz	**Abs Error**	**ratio**	**rate**
0.0025	0.000211	-	-
0.00125	9.6373e-05	2.1894	1.1305
0.000625	4.7353e-05	2.0352	1.0252
0.0003125	2.3661e-05	2.0013	1.0009

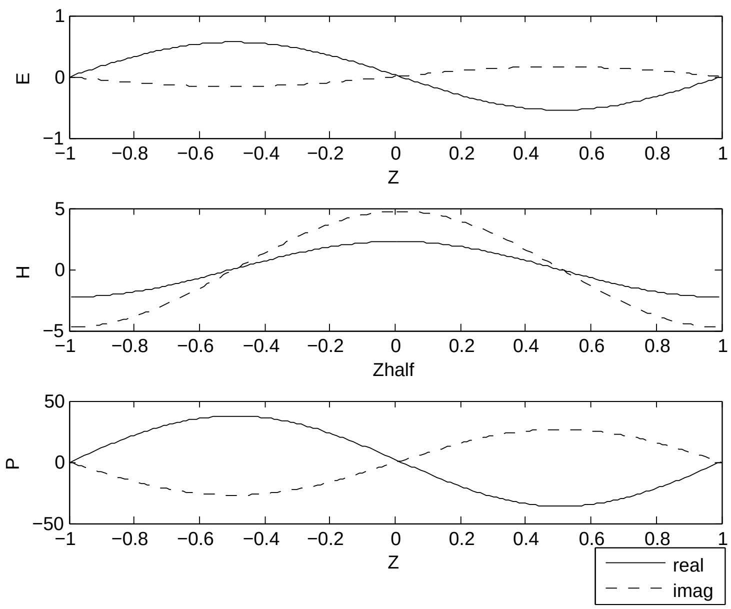


FIGURE 4.4: Final plot of exact solution in Debye media at time $t = \pi$.

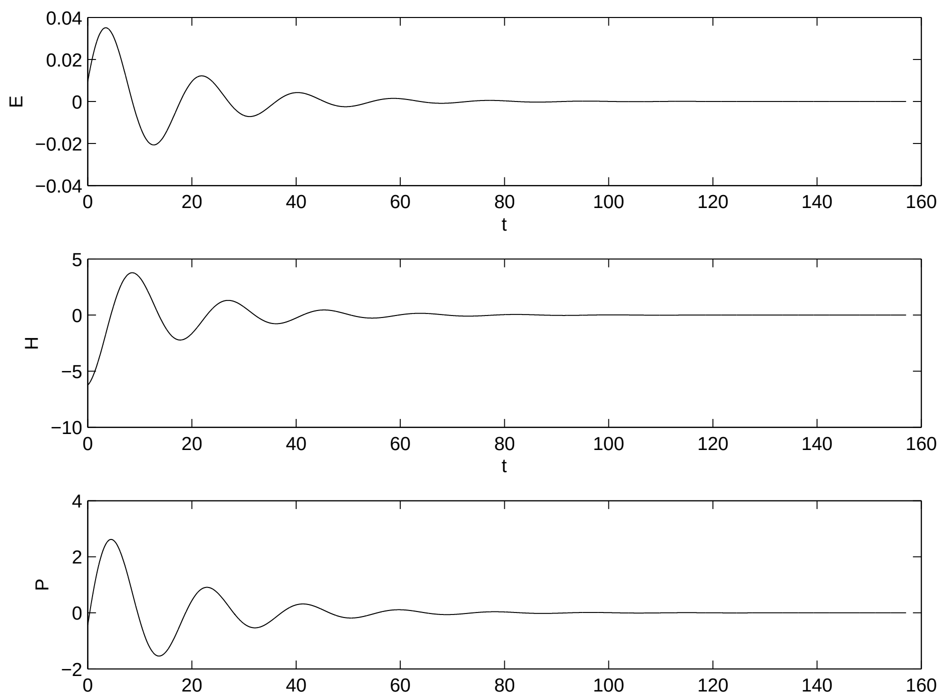


FIGURE 4.5: Time trace over $[0, 50\pi]$ at a point of depth $3\Delta z$ in the Debye media.

TABLE 4.2: Absolute error and rates of convergence with IDM modification.

Δz	**Abs Error**	**ratio**	**rate**
0.0025	0.00011332	-	-
0.00125	2.8325e-05	4.0007	2.0003
0.000625	7.0825e-06	3.9993	1.9998
0.0003125	1.77e-06	4.0014	2.0005

Yee-like FDTD schemes that are $2m\,(m > 1)$ accurate in space and second order in time, we can modify the scheme stencil locally around a material interface by introducing $2m$ fictitious points each for E, H and P, and implementing $2m$ jump conditions requiring continuity of E, H and P and their time derivatives up to order $2m - 1$ across material interfaces. We make similar assumptions on the representations of the fictitious values for the three fields E, H and P, as in the IDM technique for the modification of the Yee scheme in Debye media, namely, that the electric field fictitious points are given as linear combinations of $2m$ actual electric field values. The polarization field fictitious points are given as linear combinations of $2m$ actual electric field values and $2m$ actual polarization values. Finally, the magnetic field fictitious values are given as linear combinations of $2m$ actual electric field, polarization field and magnetic field values. This assumption leads to a block lower triangular matrix system of size $(3 \times 2m) \times (3 \times 2m)$ for the representation coefficients for the fictitious values of E, H and P. We note that even though the size of this system for the fictitious points grows with the order of the scheme, this system has to be solved just once in a pre-processing stage to obtain the representation coefficients. After this solve, the finite difference stencil is locally modified using the representation coefficients. This is as opposed to, for example, the Block Pseudospectral method [9], in which the fictitious values are solved for at every time step of the finite difference scheme.

5. CONCLUSIONS AND FUTURE DIRECTIONS

In this thesis we have successfully implemented an extension of the IDM technique [21] to dispersive media of Debye type. In such media, an additional evolution equation for the polarization vector driven by the electric field has to be appended to Maxwell's equations. The discretization of Maxwell's equations along with this evolution equation is called the auxiliary differential equation (ADE) approach [3]. The addition of the polarization field requires modification of the IDM technique as implemented for dielectrics. In particular, we require continuity of the polarization field and its time derivatives across material interfaces in addition to the continuity of the electric and magnetic field and their time derivatives across interfaces. The presence of zero order terms presents additional complications. In particular the representation coefficients for the fictitious electric, magnetic and polarization field values are no longer decoupled from those of the fictitious values of the other fields. We locally modified the Yee scheme stencil using the IDM technique and showed how second order accuracy is regained by simulating a problem with material interfaces. In the conclusions of Chapter 4 we give an idea of how this technique can be extended to locally modify the stencils of higher order in space and second order in time finite difference methods for Debye media.

We expect similar additional requirements will need to be satisfied for other types of dispersive media such as Lorentz media, Drude media, and cold plasma, among others. Media specific requirements will probably be needed in this process. For future work it will be important to consider the stability, and convergence analysis of the IDM technique as applied to $2m$ order accurate in space and second order in time finite difference schemes for Debye media.

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