

A Sequential Operator Splitting Method for Electromagnetic Wave Propagation in Dispersive Media

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Abstract

In this report we consider the Debye model along with Maxwell's equations (Maxwell-Debye) to model electromagnetic wave propagation in dispersive media that exhibit orientational polarization. We construct and analyze a sequential operator splitting method for the discretization of the Maxwell-Debye system. Energy analysis indicates that the operator splitting scheme is unconditionally stable. We also conduct a truncation error analysis to show that the scheme is first order accurate in time and second order accurate in space. We compare the operator splitting method to the Yee scheme for discretizing the Maxwell-Debye system via stability, dispersion, and dissipation analyses. Numerical simulations validate the unconditional stability of the scheme.

Keywords: Maxwell's equations, Debye media, FDTD (Yee) scheme, Operator splitting, Stability, Dispersion, Energy decay

MSC: 65M06, 65M10, 78M20

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1 Introduction

In this report we study electromagnetic wave propagation in dispersive materials that exhibit orientational polarization, by numerically discretizing Maxwell's equations along with the Debye model [5], which describes the evolution of the macroscopic polarization vector forced by the electric field [2, 3]. We will call this system the Maxwell-Debye system. We construct and analyze a sequential operator splitting (OS) method [8] for the one-dimensional Maxwell-Debye system. We conduct analysis of the OS scheme for accuracy, dispersion, dissipation, and stability, and we perform comparisons with the standard Yee or FDTD scheme [11, 10]. The main result of this research is the development of a numerical method for the Maxwell-Debye system that is unconditionally stable, allowing for independent selection of time and spatial steps based on accuracy requirements alone and not subject to stability restrictions.

In Section 2, we present the Maxwell-Debye system in three dimensions and its reductions to one and two dimensions. In Section 3, we present the Yee scheme and the implicit Crank-Nicolson scheme in one dimension for simulating wave propagation in a non-dispersive dielectric. In Section 4, we present a sequential operator splitting scheme for the one-dimensional Maxwell-Debye system. We analyze this method for accuracy, stability, and quantify dissipation and dispersion errors numerically. In particular, we prove the unconditional stability of this scheme using energy analysis. Finally, Section 5 outlines conclusions and future work.

2 Model Formulation

2.1 Maxwell's Equations

The propagation of electromagnetic waves is described by the time dependent Maxwell's equations in terms of the field variables: electric field, \mathbf{E} , magnetic field, \mathbf{H} , electric displacement, \mathbf{D} , and magnetic flux density, \mathbf{B} [1]. In a three dimensional domain $\Omega \subset \mathbb{R}^3$, and in the time interval from 0 to T , the equations are given as

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}, \quad (2.1a)$$

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E}, \quad (2.1b)$$

$$\nabla \cdot \mathbf{D} = \rho, \quad (2.1c)$$

$$\nabla \cdot \mathbf{B} = 0, \quad (2.1d)$$

along with initial conditions. We will assume perfect conducting boundary conditions on the boundary $\Gamma = \partial\Omega$ given as

$$\mathbf{n} \times \mathbf{E} = 0, \text{ on } \Gamma \times [0, T], \quad (2.2)$$

which implies that the tangential component of the electric field is zero on Γ for all time t . The field variable $\mathbf{J} = \mathbf{J}_c + \mathbf{J}_s$ comprises of the current density \mathbf{J}_c , and the source density \mathbf{J}_s . The variable ρ is called the charge density. Furthermore, the field variables can be related

by the constitutive relations which are needed to complete the system. These are

$$\mathbf{D} = \epsilon_0 \epsilon_\infty \mathbf{E} + \mathbf{P}, \quad (2.3a)$$

$$\mathbf{B} = \mu_0 \mathbf{H}, \quad (2.3b)$$

$$\mathbf{J}_c = \sigma \mathbf{E}, \quad (2.3c)$$

where the coefficients ϵ_∞ , and σ are dependent on the material through which the wave is propagating: The parameter $\epsilon_0 = 8.85418782 \times 10^{-12}$ is the electric permittivity of free space, $\mu_0 = 1.25663706 \times 10^{-6}$ the magnetic permeability of free space, and ϵ_∞ is the relative electric permittivity of the medium at infinite frequency. The speed of light in the material is $c_\infty = \frac{1}{\sqrt{\mu_0 \epsilon_0 \epsilon_\infty}} = c_0 / \sqrt{\epsilon_\infty}$, where c_0 is the speed of light in free space or vacuum. The constitutive law (2.3c) is called Ohm's law and relates \mathbf{J}_c to the electric field via σ , the electric conductivity of the medium.

We neglect magnetic effects; thus the constitutive law for the magnetic flux density (2.3b) is the same as that in free space. The macroscopic electric polarization is the \mathbf{P} variable, which may be defined as the electric field induced disturbance of the charge distribution of a region. This polarization may have delayed effects, which usually have associated time constants called relaxation times. All the field variables $\mathbf{E}, \mathbf{H}, \mathbf{D}, \mathbf{B}, \mathbf{P}$, and \mathbf{J} are functions of time t and space $\mathbf{x} = (x, y, z) \in \Omega \subset \mathbb{R}^3$.

2.2 The Debye Model for Orientational Polarization

In this section we consider the Debye model for orientational polarization [5], which models the evolution of the polarization by an ordinary differential equation (ODE) that is forced by the electric field. This ODE is given as

$$\tau \frac{\partial \mathbf{P}}{\partial t} + \mathbf{P} = \epsilon_0 \epsilon_\infty (\epsilon_q - 1) \mathbf{E}, \quad (2.4)$$

with $\epsilon_q = \epsilon_s / \epsilon_\infty$, where ϵ_s and ϵ_∞ are the relative permittivities at static and infinite frequency, respectively. The parameter τ is called the relaxation time of the material. For a full discussion of the physical Debye model, see [3]. We note that \mathbf{E} and \mathbf{P} are related to the electric flux density \mathbf{D} through the constitutive law (2.3a).

In this work we will assume the case of no conductivity, i.e., we take $\sigma = 0$ ($\mathbf{J}_c = 0$). We also assume that all the parameters of the model, i.e., $\epsilon_s, \epsilon_\infty, \epsilon_q$ and τ are all constants. We combine the constitutive relations for Debye media with (2.1b) and (2.1a) to eliminate the electric displacement \mathbf{D} and the magnetic flux density \mathbf{B} . This yields the Maxwell-Debye (M-D) system

(M-D):

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \mathbf{E}, \quad (2.5)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} \mathbf{E} + \frac{1}{\tau} \mathbf{P} - \mathbf{J}_s, \quad (2.6)$$

$$\frac{\partial \mathbf{P}}{\partial t} = \frac{(\epsilon_q - 1) \epsilon_0 \epsilon_\infty}{\tau} \mathbf{E} - \frac{1}{\tau} \mathbf{P}. \quad (2.7)$$

For any field variable \mathbf{V} , its components will be represented by $\mathbf{V} = (V_x, V_y, V_z)^T$. Writing out the vector components of the curl operator in (2.5) and (2.6) yields a system of six coupled scalar equations, which are equivalent to Maxwell's curl equations in three dimensions, along with three evolution equations for the Polarization components in (2.7). This Maxwell-Debye system in scalar form is given as

(M-D)

Equations for the Magnetic Field:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} \right), \quad (2.8a)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} \right), \quad (2.8b)$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right). \quad (2.8c)$$

Equations for the Electric Field:

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} + \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_x - \frac{1}{\tau} P_x = \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - J_{s,x}, \quad (2.9a)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} + \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_y - \frac{1}{\tau} P_y = \frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - J_{s,y}, \quad (2.9b)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_z}{\partial t} + \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_z - \frac{1}{\tau} P_z = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - J_{s,z}. \quad (2.9c)$$

Equations for the Electric Polarization:

$$\frac{\partial P_x}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_x - \frac{1}{\tau} P_x, \quad (2.10a)$$

$$\frac{\partial P_y}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_y - \frac{1}{\tau} P_y, \quad (2.10b)$$

$$\frac{\partial P_z}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_z - \frac{1}{\tau} P_z. \quad (2.10c)$$

In this paper we will concern ourselves with the one-dimensional case of the Maxwell-Debye system. We first consider the reduction of the **(M-D)** system to two dimensions.

2.3 Reduction to Two Dimensions

To reduce the Maxwell-Debye system to two dimensions we make the assumption that neither the electromagnetic field excitation nor the modeled geometry has any variation in the z -direction; that is, all partial derivatives of the fields with respect to z are zero. Then the set of equations (2.8), (2.9), and (2.10) reduces to

Equations for the Magnetic Field:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_z}{\partial y} \right), \quad (2.11a)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_z}{\partial x} \right), \quad (2.11b)$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right). \quad (2.11c)$$

Equations for the Electric Field:

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} + \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_x - \frac{1}{\tau} P_x = \frac{\partial H_z}{\partial y} - J_{s,x}, \quad (2.12a)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} + \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_y - \frac{1}{\tau} P_y = -\frac{\partial H_z}{\partial x} - J_{s,y}, \quad (2.12b)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_z}{\partial t} + \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_z - \frac{1}{\tau} P_z = \frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - J_{s,z}. \quad (2.12c)$$

Equations for the Electric Polarization:

$$\frac{\partial P_x}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_x - \frac{1}{\tau} P_x, \quad (2.13a)$$

$$\frac{\partial P_y}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_y - \frac{1}{\tau} P_y, \quad (2.13b)$$

$$\frac{\partial P_z}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_z - \frac{1}{\tau} P_z. \quad (2.13c)$$

We note that the above equations decouple into two (independent) sets. The first set is called the TE mode and is represented by two electric field (E_x, E_y) and electric polarization (P_x, P_y) components and one magnetic field (H_z) component, and their evolution equations given as the system of five equations,

2D TE Maxwell-Debye:

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu_0} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right), \quad (2.14a)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_x + \frac{1}{\tau} P_x - J_{s,x}, \quad (2.14b)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} - \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_y + \frac{1}{\tau} P_y - J_{s,y}, \quad (2.14c)$$

$$\frac{\partial P_x}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_x - \frac{1}{\tau} P_x, \quad (2.14d)$$

$$\frac{\partial P_y}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E_y - \frac{1}{\tau} P_y. \quad (2.14e)$$

The remaining four equations comprise the TM mode. In a non-dispersive dielectric $P_x = P_y = 0$, $\epsilon_q = 1$ and the equations reduce to

2D TE Maxwell:

$$\frac{\partial H_z}{\partial t} = -\frac{1}{\mu_0} \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} \right), \quad (2.15a)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y} - J_{s,x}, \quad (2.15b)$$

$$\epsilon_0 \epsilon_\infty \frac{\partial E_y}{\partial t} = -\frac{\partial H_z}{\partial x} - J_{s,y}. \quad (2.15c)$$

2.4 Reduction to One Dimension

Finally we consider the reduction of the Maxwell-Debye system to one dimension. Assuming that neither the electromagnetic field excitation nor the modeled geometry has any variation in the x and y directions, i.e., taking all derivatives with respect to x and y to be zero we have from (2.8)-(2.10) (dropping the subscripts on the variables) the system

1D Maxwell-Debye:

$$\epsilon_0 \epsilon_\infty \frac{\partial E}{\partial t} = \frac{\partial H}{\partial z} - \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E + \frac{1}{\tau} P - J_s \quad (2.16a)$$

$$\frac{\partial H}{\partial t} = \frac{1}{\mu_0} \frac{\partial E}{\partial z}, \quad (2.16b)$$

$$\frac{\partial P}{\partial t} = \frac{\epsilon_0 \epsilon_\infty (\epsilon_q - 1)}{\tau} E - \frac{1}{\tau} P, \quad (2.16c)$$

where the components $E = E_y, P = P_y$ oscillate in the (y, z) plane and propagate in the z direction, and the component $H = H_x$ oscillates in the (x, z) plane and propagates in the z direction.

In a non-dispersive dielectric $P_y = 0$ and we have a system of only two equations, which we write by dropping the subscripts on the variables, i.e., for $E = E_y, H = H_x$, we have

1D Maxwell:

$$\frac{\partial E}{\partial t} = \frac{1}{\epsilon_0 \epsilon_\infty} \frac{\partial H}{\partial z} - J_s, \quad (2.17a)$$

$$\frac{\partial H}{\partial t} = \frac{1}{\mu_0} \frac{\partial E}{\partial z}. \quad (2.17b)$$

We note that for the one-dimensional systems we lose the the Gauss divergence laws (2.1c) and (2.1d). To construct numerical methods we will discretize the Maxwell curl equations and the ODE for the Polarization .

3 Numerical Methods for the 1D Maxwell equations

We start with the 1D Maxwell equations in a non-dispersive dielectric i.e., (2.17), and consider two numerical methods for their discretization: the (explicit) staggered Yee scheme and the (implicit) Crank-Nicolson method.

3.1 Yee Scheme

The key feature of the Yee scheme is the staggering in space and time of the components of the electric field E and the magnetic field H . Let the spatial domain be $\Omega = [0, 1]$, and the time interval $[0, T], T > 0$. Let $\Delta t > 0$ and $h = \Delta z > 0$ be the time step and mesh step size, respectively, for the discretization. We define temporal nodes $t_n = n\Delta t$, where $n \geq 0$ is an integer for the electric field E and integer plus half for the magnetic field H . We define spatial nodes $z_j = jh$, where $j \geq 0$ is an integer for the electric field E , and integer plus half for the magnetic field H . Let $V_j^n \approx V(t_n, z_j)$ where V is one of the field variables E or H . Then define

$$\bar{V}_j^n = \frac{1}{2} \left(V_j^{n+1/2} + V_j^{n-1/2} \right), \quad (3.1)$$

$$\delta_z V_{j+1/2}^n = \frac{1}{\Delta z} \left(V_{j+1}^n - V_j^n \right), \quad (3.2)$$

$$\delta_t V_j^{n+1/2} = \frac{1}{\Delta t} \left(V_j^{n+1} - V_j^n \right). \quad (3.3)$$

The Yee scheme applied to the equations (2.17a) and (2.17b) uses centered differences, and takes the form of the explicit updates (assume $J_s = 0$)

(Yee):

$$E_j^{n+1} = E_j^n + \frac{1}{\varepsilon_0 \epsilon_\infty} \frac{\Delta t}{\Delta z} \left(H_{j+1/2}^{n+1/2} - H_{j-1/2}^{n+1/2} \right), \quad (3.4)$$

$$H_{j+1/2}^{n+1/2} = H_{j+1/2}^{n-1/2} + \frac{1}{\mu_0} \frac{\Delta t}{\Delta z} \left(E_{j+1}^n - E_j^n \right). \quad (3.5)$$

Given two sets of starting values, E^n and $H^{n-1/2}$ at all the spatial nodes, we can solve this explicit method for any future time step. We can compute H at time $t_{n+3/2}$ as

$$H_{j+1/2}^{n+3/2} = H_{j+1/2}^{n+1/2} + \frac{1}{\mu_0} \frac{\Delta t}{\Delta z} \left(E_{j+1}^{n+1} - E_j^{n+1} \right), \quad (3.6)$$

into which we can substitute (3.4) and (3.5) to get a unified equation,

$$H_{j+1/2}^{n+3/2} = H_{j+1/2}^{n+1/2} + \frac{1}{\mu_0} \frac{\Delta t}{\Delta z} \left[\left(E_{j+1}^n - E_j^n \right) + \frac{1}{\varepsilon_0 \epsilon_\infty} \frac{\Delta t}{\Delta z} \left(H_{j+3/2}^{n+1/2} - 2H_{j+1/2}^{n+1/2} + H_{j-1/2}^{n+1/2} \right) \right]. \quad (3.7)$$

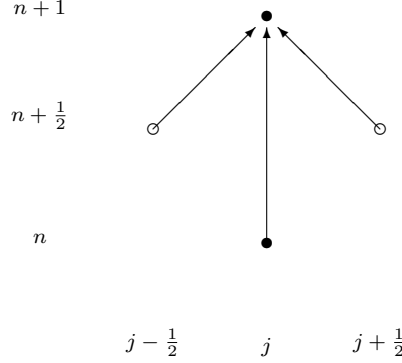
The computational stencil for the Yee scheme is given in Figure 1.

3.1.1 Accuracy of Yee Scheme

To determine the order of accuracy of the Yee scheme (3.4) - (3.5), we will use Taylor expansions to compute the local truncation error. We have the result

Lemma 3.1 ((Truncation Error)). *Assume that the solutions to the one-dimensional Maxwell's equations (2.17a) and (2.17b) are smooth enough, i.e., $E \in C^3([0, T]; C^3(\bar{\Omega}))$ and $H \in$*

Figure 1: *Computational Stencil for the Yee Scheme: The E field [solid circle] at time t_{n+1} and spatial node z_j uses the value of E at time t_n and spatial node z_j and the values of H [open circle] at spatial node $z_{j+1/2}$ and $z_{j-1/2}$ at time $t_{n+1/2}$.*



$C^3([0, T]; C^3(\bar{\Omega}))$. Let $(\tau_E)^{n+1/2}$ and $(\tau_H)^n$ denote the truncation errors of the Yee scheme equations (3.4) and (3.5), respectively. Then the truncation errors can be bounded by

$$\max_n \left\{ \left| \tau_E^{n+1/2} \right|, \left| \tau_H^n \right| \right\} \leq c(\epsilon_0, \epsilon_\infty, \mu_0)(\Delta t^2 + \Delta z^2), \quad (3.8)$$

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

Proof. Consider first (3.4). We rewrite this equation in a form that directly models the equation (2.17a) as

$$\delta_t E_j^{n+1/2} = \frac{1}{\epsilon_0 \epsilon_\infty} \delta_z H_j^{n+1/2}.$$

The local truncation error related to this discrete equation is

$$(\tau_E^{n+1/2})_j = \frac{1}{\Delta t} (E(t_{n+1}, z_j) - E(t_n, z_j)) - \frac{1}{\epsilon_0 \epsilon_\infty \Delta z} (H(t_{n+1/2}, z_{j+1/2}) - H(t_{n+1/2}, z_{j-1/2})). \quad (3.9)$$

Taking a Taylor expansion around $(t_{n+1/2}, z_j)$ and using (2.17a) the local truncation error simplifies to

$$(\tau_E)^{n+1/2})_j = \frac{\Delta t^2}{24} \frac{\partial^3 E}{\partial t^3}(\zeta_1, z_j) + \frac{\Delta z^2}{24 \epsilon_0 \epsilon_\infty} \frac{\partial^3 H}{\partial z^3}(t_n, \xi_1), \quad (3.10)$$

where $t_n < \zeta_1 < t_{n+1}$, and $z_{j-1/2} < \xi_1 < z_{j+1/2}$.

The second equation of the Yee scheme can be analyzed analogously, with Taylor expansion around $(t_n, z_{j+1/2})$. The corresponding local truncation error can be simplified as

$$(\tau_H^n)_{j+1/2} = \frac{\Delta t^2}{24} \frac{\partial^3 H}{\partial t^3}(\zeta_2, z_{j+1/2}) + \frac{\Delta z^2}{24 \mu_0} \frac{\partial^3 E}{\partial z^3}(t_n, \xi_2) \quad (3.11)$$

where $t_{n-1/2} < \zeta_2 < t_{n+1/2}$, and $z_j < \xi_2 < z_{j+1}$. The inequality (3.8) follows from the local truncation errors (3.10) and (3.11). The inequality (3.8) implies that the Yee scheme is second order accurate in space and time. \square

3.1.2 Stability of Yee Scheme

To conduct stability analysis we consider plane wave solutions. Assume that the numerical approximation of any field variable V computed by the Yee scheme has the following spatial dependence on the wave number k ,

$$V_j^n = \hat{V}^n(k)e^{ikz_j}, \quad (3.12)$$

where $V = E, H$, and the complex number $i = \sqrt{-1}$. We substitute these expressions for E and H into (3.4) and (3.7) to yield the system

$$\hat{E}^{n+1} = \hat{E}^n + \frac{1}{\varepsilon_0 \epsilon_\infty} \frac{\Delta t}{\Delta z} \left(2i \sin \left(\frac{k \Delta z}{2} \right) \right) \hat{H}^{n+1/2}, \quad (3.13)$$

$$\hat{H}^{n+3/2} = \hat{H}^{n+1/2} + \frac{1}{\mu_0} \frac{\Delta t}{\Delta z} \left(2i \sin \left(\frac{k \Delta z}{2} \right) \right) \hat{E}^n - 4\eta_\infty^2 \sin^2 \left(\frac{k \Delta z}{2} \right) \hat{H}^{n+1/2}, \quad (3.14)$$

where the speed of light in a non-dispersive dielectric, c_∞ , and the Courant number, η_∞ , are defined as

$$c_\infty = \frac{1}{\sqrt{\mu_0 \varepsilon_0 \epsilon_\infty}}, \quad (3.15)$$

$$\eta_\infty = c_\infty \frac{\Delta t}{\Delta z}. \quad (3.16)$$

Defining the parameter α as

$$\alpha = \sin \left(\frac{k \Delta z}{2} \right), \quad (3.17)$$

we can write the system (3.13)-(3.14) in matrix-vector form as

$$\begin{pmatrix} \hat{H}^{n+3/2} \\ \hat{E}^{n+1} \end{pmatrix} = \begin{bmatrix} 1 - 4\eta_\infty^2 \alpha^2 & \frac{2i\alpha\eta_\infty}{\mu_0 c_\infty} \\ \frac{2i\alpha\eta_\infty}{c_\infty \varepsilon_0 \epsilon_\infty} & 1 \end{bmatrix} \begin{pmatrix} \hat{H}^{n+1/2} \\ \hat{E}^n \end{pmatrix}. \quad (3.18)$$

The eigenvalues of the amplification matrix of system (3.18) are determined by the roots of its characteristic polynomial

$$(\lambda - 1)^2 + 4\eta_\infty^2 \alpha^2 (\lambda - 1) + 4\alpha^2 \eta_\infty^2 = 0. \quad (3.19)$$

Solving for the roots yields the eigenvalues $\lambda = 1 - 2(\eta_\infty \alpha)^2 \pm 2\sqrt{\eta_\infty^4 \alpha^4 - \eta_\infty^2 \alpha^2}$ of the amplification matrix of system (3.18). A necessary condition for stability is that all the eigenvalues of the amplification matrix must be less than or equal to one in magnitude (the von Neumann condition [9, 6]). It can easily be shown [6] that if the (Courant-Friedrichs-Lewy (CFL)) condition $\eta_\infty \leq 1$ holds, then the von Neumann condition is satisfied. The timestep Δt , as specified by the maximum CFL limit $\eta_\infty = 1$, is known as the *magic time step* for the Yee scheme, and yields the exact solution to the wave problem. However, instabilities can arise for this case as is demonstrated in [6].

3.2 An Implicit Method: The Crank Nicolson Scheme

In this section we consider an implicit method for the discretization of the 1D Maxwell's equations in a non-dispersive dielectric given in (2.17). We develop the scheme, and perform numerical simulations.

3.2.1 Formulation

With a change of variables $\tilde{E} = \sqrt{\frac{\epsilon_0 \epsilon_\infty}{\mu_0}} E$ the system (2.17) may be rewritten as (by dropping the tilde above \tilde{E})

$$\frac{\partial E}{\partial t} = c_\infty \frac{\partial H}{\partial z} - c_\infty J_s, \quad (3.20)$$

$$\frac{\partial H}{\partial t} = c_\infty \frac{\partial E}{\partial z}. \quad (3.21)$$

We construct an implicit Crank-Nicolson (C-N) numerical method by averaging terms involved in the spatial derivatives as (assume $J_s = 0$)

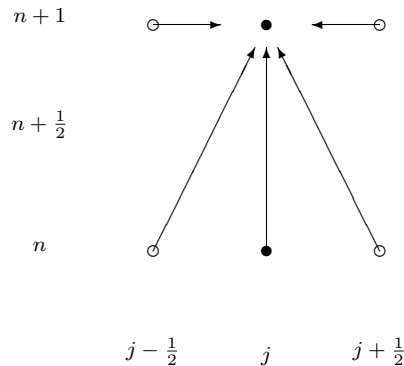
(CN):

$$\frac{E_j^{n+1} - E_j^n}{\Delta t} = c_\infty \delta_z \left(\frac{H_j^{n+1} + H_j^n}{2} \right), \quad (3.22)$$

$$\frac{H_{j+1/2}^{n+1} - H_{j+1/2}^n}{\Delta t} = c_\infty \delta_z \left(\frac{E_{j+1/2}^{n+1} + E_{j+1/2}^n}{2} \right). \quad (3.23)$$

As opposed to the conditionally stable Yee scheme, this implicit scheme is unconditionally stable. The computational stencil for this scheme is given in Figure 2. This method does

Figure 2: *Computational Stencil for the Implicit Method, showing updating of E [solid circle] using H [open circle]. Note, there is no staggering in time.*



not stagger the E and H variables in time, as the Yee scheme does. However, the scheme does stagger the E and H components in space.

The scheme (3.22), (3.23) can be written as a tridiagonal matrix system of the form $\mathbf{AX} = \mathbf{b}$ by performing the following steps. The approximations of the first order derivative in the right hand sides of equations (3.22) and (3.23) can be expanded as

$$\delta_z \left(\frac{H_j^{n+1} + H_j^n}{2} \right) = \frac{1}{2\Delta z} (H_{j+1/2}^{n+1} - H_{j-1/2}^{n+1} + H_{j+1/2}^n - H_{j-1/2}^n), \quad (3.24)$$

$$\delta_z \left(\frac{E_{j+1/2}^{n+1} + E_{j+1/2}^n}{2} \right) = \frac{1}{2\Delta z} (E_{j+1}^{n+1} - E_j^{n+1} + E_{j+1}^n - E_j^n). \quad (3.25)$$

Using the expansion (3.25) in the equation (3.23) yields the equation

$$H_{j+1/2}^{n+1} = H_{j+1/2}^n + \frac{\eta_\infty}{2} (E_{j+1}^{n+1} - E_j^{n+1} + E_{j+1}^n - E_j^n), \quad (3.26)$$

while using the expansion (3.24) in the equation (3.22) yields

$$E_i^{n+1} - E_i^n = \frac{\eta_\infty}{2} (H_{i+1/2}^{n+1} - H_{i-1/2}^{n+1} + H_{i+1/2}^n - H_{i-1/2}^n). \quad (3.27)$$

Substituting equation (3.26) into (3.27) we obtain the following equation for the electric field;

$$E_j^{n+1} \left(1 + \frac{\eta_\infty^2}{4} \right) - \frac{\eta_\infty^2}{4} (E_{j+1}^{n+1} + E_{j-1}^{n+1}) = E_j^n + \eta_\infty (H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}) + \frac{\eta_\infty^2}{4} (E_{j+1}^n - 2E_j^n + E_{j-1}^n). \quad (3.28)$$

Collecting equation (3.28) for all spatial nodes z_j we obtain the tridiagonal matrix system $\mathbf{AX} = \mathbf{b}$,

$$\begin{pmatrix} 1 & 0 & \dots & 0 & 0 \\ -\frac{\eta_\infty^2}{4} & 1 + \frac{\eta_\infty^2}{4} & -\frac{\eta_\infty^2}{4} & 0 & 0 \\ 0 & \ddots & \ddots & \ddots & 0 \\ 0 & 0 & -\frac{\eta_\infty^2}{4} & 1 + \frac{\eta_\infty^2}{4} & -\frac{\eta_\infty^2}{4} \\ 0 & 0 & \dots & 0 & 1 \end{pmatrix} \begin{pmatrix} E_0^{n+1} \\ E_1^{n+1} \\ \vdots \\ E_{M-1}^{n+1} \\ E_M^{n+1} \end{pmatrix} = \begin{pmatrix} 0 \\ b_1 \\ \vdots \\ b_{M-1} \\ 0 \end{pmatrix}, \quad (3.29)$$

where $\mathbf{X} = [E_0^{n+1}, E_1^{n+1}, \dots, E_j^{n+1}, \dots, E_{M-1}^{n+1}, E_M^{n+1}]^T$, with $M + 1$ the number of spatial nodes. The right hand side vector \mathbf{b} has the form $b = [0, b_1, \dots, b_j, \dots, b_{M-1}, 0]^T$, where for $1 \leq j \leq M - 1$,

$$b_j = E_j^n + \eta_\infty (H_{j+\frac{1}{2}}^{n+\frac{1}{2}} - H_{j-\frac{1}{2}}^{n+\frac{1}{2}}) + \frac{\eta_\infty^2}{4} (E_{j+1}^n - 2E_j^n + E_{j-1}^n). \quad (3.30)$$

The perfect conducting boundary condition $\mathbf{n} \times \mathbf{E} = 0$ translates to $E_0^n = E_M^n = 0, \forall n \geq 0$, which is reflected in the first and last entries of \mathbf{b} being zero.

3.2.2 Simulations

The implicit scheme, like the Yee scheme, is also second order accurate in space and time. We illustrate second-order accuracy and convergence to the true solution numerically. We

consider the analytic solution presented in [4]. Assume that the magnetic field H has the harmonic form $e^{i(\omega t - kz)}$, where ω is the angular frequency and k is the wave number. To satisfy Maxwell's equations (3.20)-(3.21), the electric field E should have the form $-\frac{kc_\infty}{\omega}e^{i(\omega t - kz)}$, where ω and k satisfy the dispersion relation $\omega^2 = c_\infty^2 k^2$.

Consider the domain $\Omega = [0, 1]$ with perfect conducting boundaries, i.e., $E(t, 0) = E(t, 1) = 0, \forall t \in [0, T]$, with $T = 1$. On this domain we have the analytic solution

$$E = \frac{kc_\infty}{\omega} \cos(\omega\pi t) \sin(k\pi z), \quad (3.31)$$

$$H = \sin(\omega\pi t) \cos(k\pi z). \quad (3.32)$$

Let us assume that $\epsilon_0 = \epsilon_\infty = \mu_0 = 1$. This implies that both $c_0 = 1$ and $c_\infty = 1$. The energy of the solution $(E, H)^T$ can be shown to satisfy the identity

$$\mathcal{E}(t) = \left(\int_{\Omega} \{|E(t, z)|^2 + |H(t, z)|^2\} dz \right)^{1/2} = \frac{1}{\sqrt{2}}, \quad (3.33)$$

$\forall t \in [0, T]$. With a mesh step size of $\Delta z = 1/M$, we divide the spatial domain $\Omega = [0, 1]$ into M subintervals with $M + 1$ spatial nodes. With a time step of $\Delta t = 1/N$ we divide the time interval $[0, T]$ into N sub-intervals. We recall the definition of the Courant number $\eta_\infty = c_\infty \Delta t / \Delta z = M/N$. We will specify N and η_∞ , which specifies M . Since the method is unconditionally stable the time step and mesh step size are not related by a stability condition. Thus, the parameter η_∞ is restricted by accuracy requirements only.

We define the relative error in the numerical solution as

$$\text{Rel.Err.} = \max_{0 \leq n \leq N} \left(\|E(t_n) - E^n\|_0^2 + \|H(t_n) - H^n\|_{\frac{1}{2}}^2 \right)^{1/2} / \mathcal{E}(t_n), \quad (3.34)$$

where the discrete L^2 energy norms are defined as

$$\|E^n\|_0 := \left(\Delta z \sum_{i=0}^M |E_i^n|^2 \right)^{1/2}, \quad (3.35)$$

$$\|H^n\|_{\frac{1}{2}} := \left(\Delta z \sum_{i=0}^{M-1} \left| H_{i+\frac{1}{2}}^n \right|^2 \right)^{1/2}. \quad (3.36)$$

Table 1 displays the relative errors for $\eta_\infty = 0.5$ and Table 2 displays the relative errors for $\eta_\infty = 2.0$. The ratio of errors indicate the second order accuracy of the method, while the values of η_∞ indicate the unconditional stability of the Crank Nicolson method.

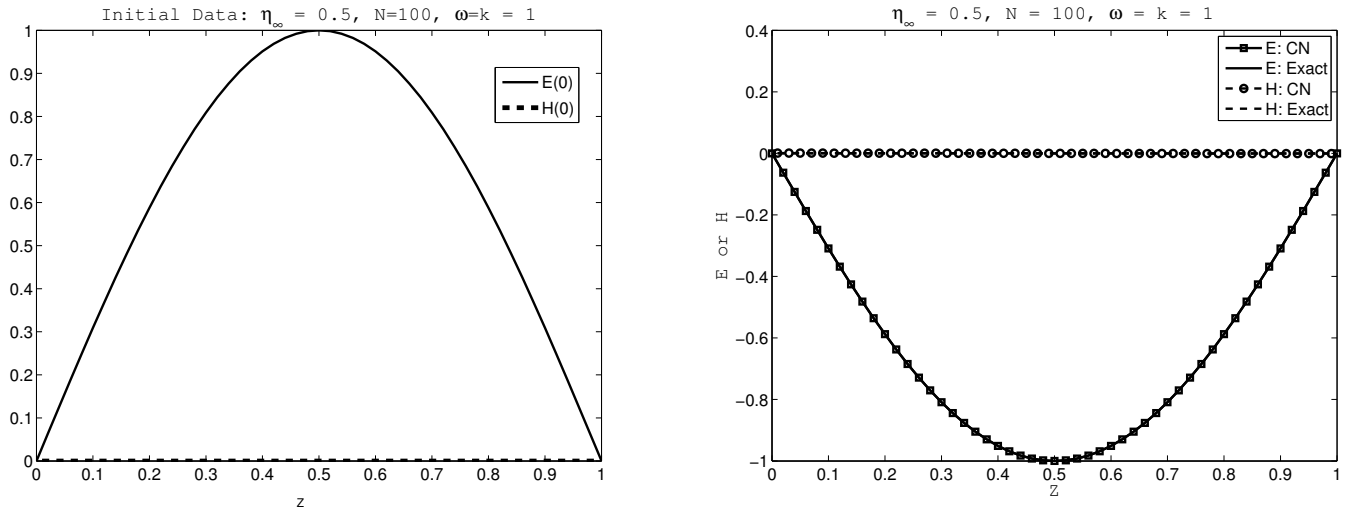
Table 1: Relative Errors for the Implicit Method. Parameters: $T = 1, \Delta t = 1/N, \eta_\infty = 0.5, \Delta z = \Delta t/\eta_\infty, \omega = k = 1$.

N	Δt	Δz	Rel.Err.	Ratio of Errors
50	0.02	0.04	0.0031	
100	0.01	0.02	7.7497e-04	4.0002
200	0.005	0.01	1.9378e-04	3.9992
400	0.0025	0.005	4.8447e-05	3.9998

Table 2: Relative Errors for the Implicit Method. Parameters: $T = 1, \Delta t = 1/N, \eta_\infty = 2.0, \Delta z = \Delta t/\eta_\infty, \omega = k = 1$.

N	Δt	Δz	Rel.Err.	Ratio of Errors
50	0.02	0.01	0.0012	
100	0.01	0.005	2.9064e-04	4.1288
200	0.005	0.0025	7.2668e-05	3.9996
400	0.0025	0.0013	1.8168e-05	3.9998

Figure 3: Exact and Crank-Nicolson (CN) Numerical Solutions for $N = 100, \eta_\infty = 0.5, \omega = k = 1$. The left plot shows the initial data, while the right plot shows the solutions at $T = 1.0$.



4 A Sequential Operator Splitting Method for Maxwell-Debye Media

4.1 Formulation

In this section we construct a sequential operator splitting scheme for the 1D Maxwell-Debye system given in equations (2.16a)-(2.16c). We scale the equations (2.16a), (2.16b),

and (2.16c) using the change of variables $\tilde{E} = \sqrt{\frac{\varepsilon_0 \varepsilon_\infty}{\mu_0}} E$, to obtain a modified system which can be rewritten as (dropping the tilde for convenience)

1D Maxwell-Debye:

$$\frac{\partial H}{\partial t} = c_\infty \frac{\partial E}{\partial z}, \quad (4.1a)$$

$$\frac{\partial E}{\partial t} = c_\infty \frac{\partial H}{\partial z} - \frac{\varepsilon_q - 1}{\tau} E + \frac{c_\infty}{\tau} P - c_\infty J_s, \quad (4.1b)$$

$$\frac{\partial P}{\partial t} = \frac{\varepsilon_q - 1}{c_\infty \tau} E - \frac{1}{\tau} P. \quad (4.1c)$$

Define $\mathbf{U} = [H, E, P]^T$. Using this definition, we can rewrite system (4.1) in matrix form as

$$\frac{\partial \mathbf{U}}{\partial t} = \begin{pmatrix} 0 & c_\infty \frac{\partial}{\partial z} & 0 \\ c_\infty \frac{\partial}{\partial z} & \frac{-(\varepsilon_q - 1)}{\tau} & \frac{c_\infty}{\tau} \\ 0 & \frac{(\varepsilon_q - 1)}{c_\infty \tau} & -\frac{1}{\tau} \end{pmatrix} \mathbf{U} + \begin{pmatrix} 0 \\ -c_\infty J_s \\ 0 \end{pmatrix}. \quad (4.2)$$

To construct a sequential operator splitting scheme we write the matrix operator in (4.2) as a sum of two operators,

$$\frac{\partial \mathbf{U}}{\partial t} = \frac{1}{\tau} \mathcal{A} \mathbf{U} + \mathcal{B} \mathbf{U} + \mathcal{J}_s, \quad (4.3)$$

where,

$$\mathcal{A} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & -(\varepsilon_q - 1) & c_\infty \\ 0 & \frac{\varepsilon_q - 1}{c_\infty} & -1 \end{pmatrix}; \quad \mathcal{B} = \begin{pmatrix} 0 & c_\infty \frac{\partial}{\partial z} & 0 \\ c_\infty \frac{\partial}{\partial z} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad \mathcal{J} = \begin{pmatrix} 0 \\ -c_\infty J_s \\ 0 \end{pmatrix} \quad (4.4)$$

This splitting separates terms involving τ , the relaxation time, from other terms. We will call the operator \mathcal{A} as the stiff operator and \mathcal{B} as the non-stiff operator.

Given the time step $\Delta t > 0$, for integer $n \geq 0$, let $\mathbf{U}^n \approx \mathbf{U}(t_n, \cdot)$. The sequential operator splitting scheme does the following:

(SS): Given $\mathbf{U}^0 = [H^0, E^0, P^0]^T$

for $n = 0$ to $N - 1$

(S1) Solve for $\tilde{\mathbf{U}}^{n+1} = [\tilde{H}^{n+1}, \tilde{E}^{n+1}, \tilde{P}^{n+1}]^T$ on (t_n, t_{n+1}) in

$$\frac{\partial \tilde{\mathbf{U}}}{\partial t} = \mathcal{B} \tilde{\mathbf{U}} + \mathcal{J}; \quad \tilde{\mathbf{U}}(t_n) = \mathbf{U}^n \quad (4.5)$$

(S2) Solve for $\mathbf{U}^{n+1} = [H^{n+1}, E^{n+1}, P^{n+1}]^T$ on (t_n, t_{n+1}) in

$$\frac{\partial \mathbf{U}}{\partial t} = \frac{1}{\tau} \mathcal{A} \mathbf{U}; \quad \mathbf{U}(t_n) = \tilde{\mathbf{U}}^{n+1} \quad (4.6)$$

end

The sub-steps (S1) and (S2) communicate through their initial conditions. The solution of (S1) becomes the initial condition for (S2) and the solution of (S2) then is the initial data

for (S1). We discretize sub-step (S1) of the **(SS)** scheme using the Crank Nicholson **(CN)** scheme for a non-dispersive dielectric that was presented in Section 3.2, since in this sub-step the polarization vector does not change. The sub-step (S2) is also discretized in an implicit manner.

(SS-D): Given $\mathbf{U}^0 = [H^0, E^0, P^0]^T$
for $n = 0$ to $N - 1$

(S1) Solve for $\tilde{\mathbf{U}}^{n+1} = [\tilde{H}^{n+1}, \tilde{E}^{n+1}, \tilde{P}^{n+1}]^T$ on (t_n, t_{n+1}) in

$$\frac{\tilde{H}_{i+\frac{1}{2}}^{n+1} - H_{i+\frac{1}{2}}^n}{\Delta t} = c_\infty \delta_z \left(\frac{\tilde{E}_{i+\frac{1}{2}}^{n+1} + E_{i+\frac{1}{2}}^n}{2} \right), \quad (4.7)$$

$$\frac{\tilde{E}_i^{n+1} - E_i^n}{\Delta t} = c_\infty \delta_z \left(\frac{\tilde{H}_i^{n+1} + H_i^n}{2} \right) - c_\infty (J_s)_i^{n+\frac{1}{2}}, \quad (4.8)$$

$$\frac{\tilde{P}_i^{n+1} - P_i^n}{\Delta t} = 0. \quad (4.9)$$

(S2) Solve for $\mathbf{U}^{n+1} = [H^{n+1}, E^{n+1}, P^{n+1}]^T$ on (t_n, t_{n+1}) in

$$\frac{H_i^{n+1} - \tilde{H}_i^{n+1}}{\Delta t} = 0, \quad (4.10)$$

$$\frac{E_i^{n+1} - \tilde{E}_i^{n+1}}{\Delta t} = -\left(\frac{\epsilon_q - 1}{2\tau}\right)(E_i^{n+1} + \tilde{E}_i^{n+1}) + \frac{c_\infty}{2\tau}(P_i^{n+1} + \tilde{P}_i^{n+1}), \quad (4.11)$$

$$\frac{P_i^{n+1} - \tilde{P}_i^{n+1}}{\Delta t} = \left(\frac{\epsilon_q - 1}{2c_\infty\tau}\right)(E_i^{n+1} + \tilde{E}_i^{n+1}) - \frac{1}{2\tau}(P_i^{n+1} + \tilde{P}_i^{n+1}). \quad (4.12)$$

end

We will show that this sequential splitting gives a first order accurate scheme in time, but is second order accurate in space. Sub-step (S2) can be written as an explicit matrix-vector update. We have the following result for sub-step (S2).

Lemma 4.1. *The update equations (4.11)-(4.12) in sub-step S2 of the operator splitting scheme **(SS-D)** can be written as the matrix-vector update*

$$\mathbf{U}^{n+1} = \mathcal{C}_{\Delta t} \tilde{\mathbf{U}}^{n+1} \quad (4.13)$$

where the matrix

$$\mathcal{C}_{\Delta t} = \mathcal{I}_3 - \alpha_{\Delta t} \mathcal{A} \quad (4.14)$$

with

$$\alpha_{\Delta t} = -\frac{\Delta t}{\tau} \left(1 + \frac{\epsilon_q \Delta t}{2\tau} \right)^{-1} \quad (4.15)$$

and the matrix \mathcal{A} is as defined in (4.4).

Proof. From equations (4.11) and (4.12) collecting E and P terms at time t_{n+1} on the left hand side and terms involving the solution of sub-step (S1) on the right hand side, we can write

$$E^{n+1}\left(1 + \frac{\Delta t(\varepsilon_q - 1)}{2\tau}\right) + P^{n+1}\left(-\frac{c_\infty \Delta t}{2\tau}\right) = \tilde{E}^{n+1}\left(1 - \frac{\Delta t(\varepsilon_q - 1)}{2\tau}\right) + \tilde{P}^{n+1}\left(\frac{c_\infty \Delta t}{2\tau}\right), \quad (4.16)$$

$$P^{n+1}\left(1 + \frac{\Delta t}{2\tau}\right) + E^{n+1}\left(-\frac{\Delta t(\varepsilon_q - 1)}{2c_\infty \tau}\right) = \tilde{E}^{n+1}\left(\frac{\Delta t(\varepsilon_q - 1)}{2c_\infty \tau}\right) + \tilde{P}^{n+1}\left(1 - \frac{\Delta t}{2\tau}\right). \quad (4.17)$$

This can be written in matrix form as

$$\mathcal{C}_{1,\Delta t} \begin{pmatrix} E^{n+1} \\ P^{n+1} \end{pmatrix} = \mathcal{C}_{2,\Delta t} \begin{pmatrix} \tilde{E}^{n+1} \\ \tilde{P}^{n+1} \end{pmatrix}, \quad (4.18)$$

with

$$\mathcal{C}_{1,\Delta t} = \begin{pmatrix} 1 + \frac{\Delta t(\varepsilon_q - 1)}{2\tau} & -\frac{c_\infty \Delta t}{2\tau} \\ -\frac{\Delta t(\varepsilon_q - 1)}{2c_\infty \tau} & 1 + \frac{\Delta t}{2\tau} \end{pmatrix}, \quad (4.19)$$

$$\mathcal{C}_{2,\Delta t} = \begin{pmatrix} 1 - \frac{\Delta t(\varepsilon_q - 1)}{2\tau} & \frac{c_\infty \Delta t}{2\tau} \\ \frac{\Delta t(\varepsilon_q - 1)}{2c_\infty \tau} & 1 - \frac{\Delta t}{2\tau} \end{pmatrix}. \quad (4.20)$$

The matrix $\mathcal{C}_{\Delta t} = \mathcal{C}_{1,\Delta t}^{-1} \mathcal{C}_{2,\Delta t}$ is easily shown to have the form in (4.14)-(4.15). \square

4.2 Equivalent Operating Splitting Scheme (E-OS)

In order to analyze the discretized operator splitting scheme, **(SS-D)**, we introduce an equivalent scheme **(E-OS)** here. This equivalent scheme merges the two steps of the operator splitting method into one system. The equivalent scheme is obtained by eliminating the intermediate variable $\tilde{\mathbf{U}}^{n+1}$. We define the parameter $\gamma = \Delta t(\varepsilon_q - 1)$ and via some algebra arrive at the system

(E-OS):

$$\delta_t(E_j^{n+1/2}) = -\frac{2(\varepsilon_q - 1)}{2\tau - \gamma} E_j^{n+1} + c_\infty \delta_z \left(\frac{H_j^{n+1} + H_j^n}{2} \right) + \frac{c_\infty}{2\tau - \gamma} (P_j^{n+1} + P_j^n), \quad (4.21)$$

$$\delta_t(H_{j+1/2}^{n+1/2}) = \frac{c_\infty}{4\tau - 2\gamma} \delta_z \left((2\tau + \gamma) E_{j+1/2}^{n+1} - c_\infty \Delta t (P_{j+1/2}^{n+1} + P_{j+1/2}^n) + (2\tau - \gamma) E_{j+1/2}^n \right), \quad (4.22)$$

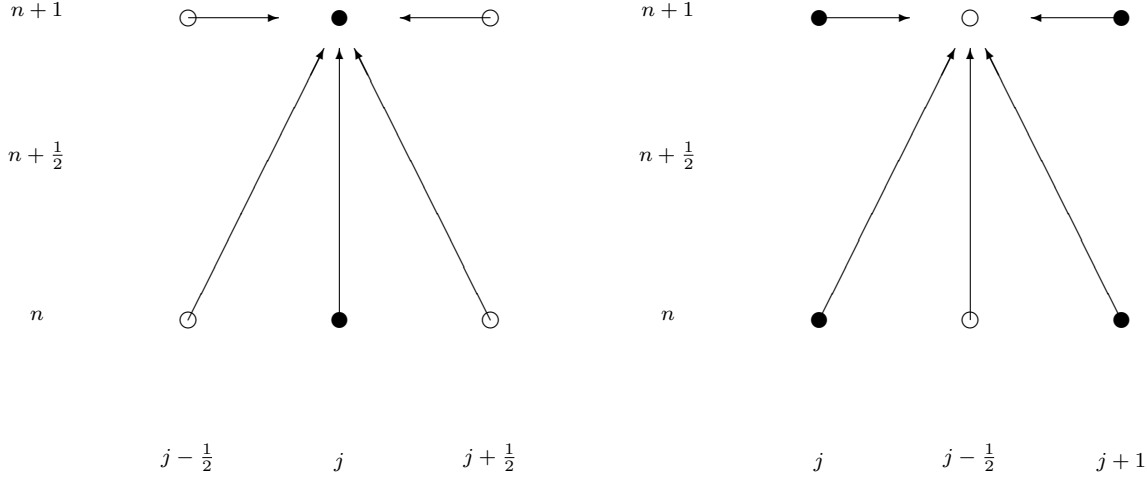
$$\delta_t(P_j^{n+1/2}) = \frac{2(\varepsilon_q - 1)}{c_\infty(2\tau - \gamma)} E_j^{n+1} - \left(\frac{1}{2\tau - \gamma} \right) (P_j^{n+1} + P_j^n). \quad (4.23)$$

The source term $J_{sj}^{n+1/2}$ is assumed to be zero. Figure 4 depicts the computational stencil for the **(E-OS)** scheme.

4.3 Truncation Error Analysis of (E-OS)

In this section, we first introduce the Crank-Nicolson **(CN-MD)** scheme for the modified 1D Maxwell-Debye system given in equations (4.1). Next, we show that the (equivalent)

Figure 4: *Computational Stencil for the equivalent operator splitting method (E-OS), showing updating of E (left) and H (right). E and P are computed at the same points [solid circle], while H is computed at staggered points in space [open circle].*



sequential operator splitting scheme (**E-OS**) is a first order in time perturbation of the (**CN-MD**) scheme, and is thus first order accurate in time, and second order accurate in space.

The Crank-Nicolson method for the 1D Maxwell-Debye system is an implicit scheme which treats the E and H terms as described in the (**CN**) scheme for a non-dispersive dielectric in Section 3.2, and averages the lower order terms in E and P . The discrete update equations for this scheme are given as

(**CN-MD**):

$$\delta_t(H_{j+1/2}^{n+1/2}) = c_\infty \delta_z \bar{E}_{j+1/2}^{n+1/2}, \quad (4.24)$$

$$\delta_t(E_j^{n+1/2}) = c_\infty \delta_z \bar{H}_j^{n+1/2} - \frac{\varepsilon_q - 1}{\tau} \bar{E}_j^{n+1/2} + \frac{c_\infty}{\tau} \bar{P}_j^{n+1/2}, \quad (4.25)$$

$$\delta_t(P_j^{n+1/2}) = \frac{\varepsilon_q - 1}{c_\infty \tau} \bar{E}_j^{n+1/2} - \frac{1}{\tau} \bar{P}_j^{n+1/2}. \quad (4.26)$$

We will denote the truncation errors of the (**CN-MD**) scheme by $\xi_H^{n+1/2}$, $\xi_E^{n+1/2}$, and $\xi_P^{n+1/2}$, respectively, with the definitions

$$\xi_{H_{j+1/2}}^{n+1/2} = \frac{1}{\Delta t} (H(t_{n+1}, z_{j+1/2}) - H(t_n, z_{j+1/2})) - \frac{c_\infty}{2} \delta_z (E(t_{n+1}, z_{j+1/2}) + E(t_n, z_{j+1/2})), \quad (4.27)$$

$$\xi_{E_j}^{n+1/2} = \frac{1}{\Delta t} (E(t_{n+1}, z_j) - E(t_n, z_j)) - \frac{c_\infty}{2} \delta_z (H(t_{n+1}, z_j) + H(t_n, z_j)) \quad (4.28)$$

$$+ \frac{\varepsilon_q - 1}{2\tau} (E(t_{n+1}, z_j) + E(t_n, z_j)) - \frac{c_\infty}{2\tau} (P(t_{n+1}, z_j) + P(t_n, z_j)), \quad (4.29)$$

$$\xi_{P_j}^{n+1/2} = \frac{1}{\Delta t} (P(t_{n+1}, z_j) - P(t_n, z_j)) - \frac{\varepsilon_q - 1}{2\tau c_\infty} (E(t_{n+1}, z_j) + E(t_n, z_j)) \quad (4.30)$$

$$+ \frac{1}{2\tau} (P(t_{n+1}, z_j) + P(t_n, z_j)) \quad (4.31)$$

Using Taylor expansions, we can show that the truncation errors are second order accurate in both space and time. We have

$$\begin{aligned} \xi_{E_j}^{n+1/2} &= \Delta t^2 \left(\frac{1}{24} \frac{\partial^3 E}{\partial t^3}(\tau_{E1}, z_j) + \frac{\epsilon_q - 1}{8\tau} \frac{\partial^2 E}{\partial t^2}(\tau_{E2}, z_j) - \frac{c_\infty}{8\tau} \frac{\partial^2 P}{\partial t^2}(\tau_{E3}, z_j) - \frac{c_\infty}{8} \frac{\partial^3 H}{\partial t^2 \partial z}(\tau_{E4}, z_{E1}) \right) \\ &\quad - \Delta z^2 \left(\frac{c_\infty}{24} \frac{\partial^3 H}{\partial z^3}(t_{n+\frac{1}{2}}, z_{E2}) \right) \end{aligned} \quad (4.32)$$

Similarly, we have

$$\xi_{H_{j+\frac{1}{2}}}^{n+1/2} = \Delta t^2 \left(\frac{1}{24} \frac{\partial^3 H}{\partial t^3}(\tau_{H1}, z_{j+\frac{1}{2}}) - \frac{c_\infty}{8} \frac{\partial^3 E}{\partial t^2 \partial z}(\tau_{H2}, z_{H1}) \right) - \Delta z^2 \left(\frac{c_\infty}{24} \frac{\partial^3 E}{\partial z^3}(t_{n+\frac{1}{2}}, z_{H2}) \right) \quad (4.33)$$

$$\xi_{P_j}^{n+1/2} = \Delta t^2 \left(\frac{1}{24} \frac{\partial^3 P}{\partial t^3}(\tau_{P1}, z_j) + \frac{1}{8\tau} \frac{\partial^2 P}{\partial t^3}(\tau_{P2}, z_j) + \frac{\epsilon_q - 1}{8c_\infty \tau} \frac{\partial^2 E}{\partial t^2}(\tau_{P3}, z_j) \right) \quad (4.34)$$

where we have $t_n \leq \tau_{E1}, \tau_{E1}, \tau_{E2}, \tau_{E3}, \tau_{E4} \leq t_{n+1/2}$, $t_n \leq \tau_{H1}, \tau_{H2} \leq t_{n+1/2}$, $t_n \leq \tau_{P1}, \tau_{P2}, \tau_{P3}, \tau_{P4} \leq t_{n+1/2}$, and $z_{j-1/2} \leq z_{E1}, z_{E2} \leq z_{j+1/2}$ and $z_j \leq z_{H1}, z_{H2} \leq z_{j+1}$. Since we can bound the errors by

$$\max \{ |\xi_E^{n+\frac{1}{2}}|, |\xi_H^{n+\frac{1}{2}}|, |\xi_P^{n+\frac{1}{2}}| \} \leq C(c_\infty, \epsilon_q, \tau)(\Delta t^2 + \Delta z^2), \quad (4.35)$$

where the constant C is independent of the mesh sizes Δt and Δz , the Crank-Nicolson scheme is second order accurate in space and time.

Lemma 4.2. *Assume that the solutions to the Maxwell-Debye system, (4.1), are smooth enough, i.e., they satisfy the regularity conditions: $E, H, P \in C^3([0, T]; [C^3(\bar{\Omega})])$. Let $\eta_E^{n+1/2}, \eta_H^{n+1/2}$, and $\eta_P^{n+1/2}$ be the truncation errors of the sequential splitting scheme **(E-OS)**. Then:*

$$\max_n \{ \eta_E^{n+1/2}, \eta_H^{n+1/2}, \eta_P^{n+1/2} \} \leq C_1(c_\infty, \tau, \epsilon_q) \{ \Delta t + \Delta z^2 \} \quad (4.36)$$

The constants C_1 and C_2 are independent of the mesh sizes Δt and Δz .

Proof. The sequential splitting scheme **(E-OS)**, (4.21, 4.22, 4.23) is a first order in time perturbation of the second order accurate in time and space Crank-Nicolson scheme **(CN-MD)**, (4.24, 4.25, 4.26). This follows from the fact that the truncation errors for the **(E-OS)** scheme can be written as

$$\eta_{H_{j+\frac{1}{2}}}^{n+1/2} = \xi_{H_{j+\frac{1}{2}}}^{n+1/2} + \Delta t \left(\frac{c_\infty(\epsilon_q - 1)}{2\tau} \delta_z E(t_{n+1}, z_{j+\frac{1}{2}}) - \frac{c_\infty^2}{4\tau} \delta_z (P(t_{n+1}, z_{j+\frac{1}{2}}) + P(t_n, z_{j+\frac{1}{2}})) \right), \quad (4.37)$$

$$\eta_{E_{j+\frac{1}{2}}}^{n+1/2} = \xi_{E_{j+\frac{1}{2}}}^{n+1/2} + \Delta t \left(\frac{c_\infty}{2\tau} P(t_{n+\frac{1}{2}}, z_j) - \frac{(\epsilon_q - 1)}{2\tau} \left(\frac{\partial E}{\partial t}(t_{n+\frac{1}{2}}, z_j) + E(t_{n+\frac{1}{2}}, z_j) \right) \right), \quad (4.38)$$

$$\eta_{P_{j+\frac{1}{2}}}^{n+1/2} = \xi_{P_{j+\frac{1}{2}}}^{n+1/2} - \Delta t \left(\frac{1}{2\tau} P(t_{n+\frac{1}{2}}, z_j) + \frac{(\epsilon_q - 1)}{2\tau c_\infty} \left(\frac{\partial E}{\partial t}(t_{n+\frac{1}{2}}, z_j) + E(t_{n+\frac{1}{2}}, z_j) \right) \right). \quad (4.39)$$

□

4.4 Stability Analysis via the Energy Method

In this section we prove that the operator splitting method (**SS-D**) is unconditional stable by demonstrating the decay of a discrete energy. We will retain the same notation as in Section 3.2 for the discrete space-time mesh. We have the result

Lemma 4.3. *Assuming perfect conducting boundary conditions, i.e., $E_0^n = 0, E_M^n = 0$, $\forall n, 0 \leq n \leq N$ we have the discrete Green's identity (integration by parts)*

$$\sum_{\ell=0}^{M-1} E_\ell^n \delta_z H_\ell^n + \sum_{\ell=0}^{M-1} (\delta_z E_{\ell+\frac{1}{2}}^n) H_{\ell+\frac{1}{2}}^n = 0. \quad (4.40)$$

Proof. Dropping the time index, i.e., $V_\ell = V_\ell^n$, for $V = E, H$, we have, using the definition of the discrete operator δ_z ,

$$\begin{aligned} \sum_{j=0}^{M-1} E_j \delta_z H_j &= \left[\sum_{j=1}^{M-1} \left(E_j H_{j+\frac{1}{2}} \right) - \sum_{j=1}^{M-1} \left(E_j H_{j-\frac{1}{2}} \right) \right] \cdot \frac{1}{\Delta z} \\ &= - \left[\sum_{\ell=0}^{M-2} \left(E_{\ell+1} H_{\ell+\frac{1}{2}} \right) - \sum_{\ell=1}^{M-1} \left(E_\ell H_{\ell+\frac{1}{2}} \right) \right] \cdot \frac{1}{\Delta z} \\ &= - \left[\sum_{\ell=0}^{M-1} \left(E_{\ell+1} H_{\ell+\frac{1}{2}} \right) - \sum_{\ell=0}^{M-1} E_\ell H_{\ell+\frac{1}{2}} \right] \cdot \frac{1}{\Delta z} \end{aligned}$$

Thus, we obtain

$$\begin{aligned} \sum_{j=0}^{M-1} E_j \delta_z H_j &= - \sum_{\ell=0}^{M-1} \left(\frac{E_{\ell+1} - E_\ell}{\Delta z} \right) H_{\ell+\frac{1}{2}} \\ &= - \sum_{\ell=0}^{M-1} \delta_z \left(E_{\ell+\frac{1}{2}} \right) H_{\ell+\frac{1}{2}}. \end{aligned}$$

Thus, the identity (4.40) follows. \square

Based on Lemma 4.3, we now prove the decay of a discrete energy for the (**SS-D**) scheme.

Theorem 4.1 ((Discrete Energy Decay)). *For the integers $n \geq 0$, let $\mathbf{U}^n = [H^n, E^n, P^n]^T$ be the solutions of the Operator Splitting Scheme (**SS-D**) with perfect conducting boundary conditions. Then there exists the energy decay property*

$$\mathcal{E}_h^{n+1} \leq \mathcal{E}_h^n \quad (4.41)$$

where, the discrete energy is defined as

$$\mathcal{E}_h^n = \left(\left\| \frac{1}{\sqrt{c_\infty}} H^n \right\|_{\frac{1}{2}}^2 + \left\| \frac{1}{\sqrt{c_\infty}} E^n \right\|_0^2 + \left\| \sqrt{\frac{c_\infty}{\epsilon_q - 1}} P^n \right\|_0^2 \right)^{1/2}, \quad (4.42)$$

and the discrete L^2 energy norms in the above are defined in equations (3.35) and (3.36).

Proof. We will again assume that the source term $J_s = 0$. Starting with sub-step (S1) of the sequential splitting scheme **(SS-D)**, we multiply (4.8) by the term $\frac{\Delta t}{c_\infty}(\tilde{E}_i^{n+1} + E_i^n)$ to get

$$\frac{1}{c_\infty} \left[\left(\tilde{E}_i^{n+1} \right)^2 - \left(E_i^n \right)^2 \right] = \frac{\Delta t}{2} \delta_z \left(\tilde{H}_i^{n+1} + H_i^n \right) \left(\tilde{E}_i^{n+1} + E_i^n \right). \quad (4.43)$$

Similarly we multiply (4.7) by $\frac{\Delta t}{c_\infty}(\tilde{H}_{i+1/2}^{n+1} + H_{i+1/2}^n)$, resulting in

$$\frac{1}{c_\infty} \left[\left(\tilde{H}_{i+1/2}^{n+1} \right)^2 - \left(H_{i+1/2}^n \right)^2 \right] = \frac{\Delta t}{2} \delta_z \left(\tilde{E}_{i+1/2}^{n+1} + E_{i+1/2}^n \right) \left(\tilde{H}_{i+1/2}^{n+1} + H_{i+1/2}^n \right). \quad (4.44)$$

Adding equations (4.43) and (4.44) together, and taking the sum over all spatial nodes in the discrete mesh we get the identity

$$\begin{aligned} \frac{1}{c_\infty} \sum_{i=0}^{M-1} \left[\left(\tilde{E}_i^{n+1} \right)^2 - \left(E_i^n \right)^2 + \left(\tilde{H}_{i+1/2}^{n+1} \right)^2 - \left(H_{i+1/2}^n \right)^2 \right] = \\ \frac{\Delta t}{2} \sum_{i=0}^{M-1} \left[\left(\tilde{E}_i^{n+1} + E_i^n \right) \delta_z \left(\tilde{H}_i^{n+1} + H_i^n \right) + \left(\tilde{H}_{i+1/2}^{n+1} + H_{i+1/2}^n \right) \delta_z \left(\tilde{E}_{i+1/2}^{n+1} + E_{i+1/2}^n \right) \right] \end{aligned} \quad (4.45)$$

By using Lemma 4.3 we can rewrite the first term of the right hand side as

$$\sum_{i=0}^{M-1} \delta_z \left(\tilde{H}_i^{n+1} + H_i^n \right) \left(\tilde{E}_i^{n+1} + E_i^n \right) = - \sum_{i=0}^{M-1} \delta_z \left(\tilde{E}_{i+1/2}^{n+1} + E_{i+1/2}^n \right) \left(\tilde{H}_{i+1/2}^{n+1} + H_{i+1/2}^n \right), \quad (4.46)$$

which implies that the right hand side of the identity (4.45) is zero. Thus, we get the identity

$$\frac{1}{c_\infty} \sum_{i=0}^{M-1} \left[\left(\tilde{E}_i^{n+1} \right)^2 - \left(E_i^n \right)^2 + \left(\tilde{H}_{i+1/2}^{n+1} \right)^2 - \left(H_{i+1/2}^n \right)^2 \right] = 0. \quad (4.47)$$

Next, we consider sub-step (S2) of **(SS-D)**. Multiplying equation (4.11) by $\bar{E}_i^{n+1} \left(\frac{\Delta t}{c_\infty} \right)$ we get

$$\frac{1}{c_\infty} \left[\left(E_i^{n+1} \right)^2 - \left(\tilde{E}_i^{n+1} \right)^2 \right] = - \frac{\Delta t (e_q - 1)}{2\tau c_\infty} \left(\bar{E}_i^{n+1} \right)^2 + \frac{\Delta t}{2\tau} \bar{P}_i^{n+1} \bar{E}_i^{n+1}. \quad (4.48)$$

Multiplying (4.12) $\bar{P}_i^{n+1} \left(\frac{c_\infty \Delta t}{e_q - 1} \right)$ we have

$$\frac{c_\infty}{e_q - 1} \left[\left(P_i^{n+1} \right)^2 - \left(\tilde{P}_i^{n+1} \right)^2 \right] = \frac{\Delta t}{2\tau} \bar{E}_i^{n+1} \bar{P}_i^{n+1} - \frac{\Delta t c_\infty}{2\tau (e_q - 1)} \left(\bar{P}_i^{n+1} \right)^2. \quad (4.49)$$

Adding (4.48) and (4.49) together, we obtain the identity

$$\begin{aligned} \frac{1}{c_\infty} \left(E_i^{n+1} \right)^2 - \frac{1}{c_\infty} \left(\tilde{E}_i^{n+1} \right)^2 + \frac{c_\infty}{e_q - 1} \left(P_i^{n+1} \right)^2 - \frac{c_\infty}{e_q - 1} \left(\tilde{P}_i^{n+1} \right)^2 \\ = - \frac{\Delta t (e_q - 1)}{2\tau c_\infty} \left(\bar{E}_i^{n+1} \right)^2 - \frac{\Delta t c_\infty}{2\tau (e_q - 1)} \left(\bar{P}_i^{n+1} \right)^2 + \frac{\Delta t}{\tau} \bar{P}_i^{n+1} \bar{E}_i^{n+1}, \end{aligned} \quad (4.50)$$

in which the right hand side can be rewritten as

$$\begin{aligned} & \frac{1}{c_\infty} (E_i^{n+1})^2 - \frac{1}{c_\infty} (\tilde{E}_i^{n+1})^2 + \frac{c_\infty}{e_q - 1} (P_i^{n+1})^2 - \frac{c_\infty}{e_q - 1} (\tilde{P}_i^{n+1})^2 \\ &= -\frac{\Delta t}{2\tau} \left[\sqrt{\frac{e_q - 1}{c_\infty}} (\bar{E}_i^{n+1}) - \sqrt{\frac{c_\infty}{e_q - 1}} (\bar{P}_i^{n+1}) \right]^2. \end{aligned} \quad (4.51)$$

Finally adding the identities (4.47) and (4.51) together, and using the fact that $\tilde{H}_{i+1/2}^{n+1} = H_{i+1/2}^{n+1}$, and $\tilde{P}_i^{n+1} = P_i^n$, we get the inequality

$$\frac{1}{c_\infty} \sum_{i=0}^{M-1} \left[(E_i^{n+1})^2 - (E_i^n)^2 + (H_{i+1/2}^{n+1})^2 - (H_{i+1/2}^n)^2 + \frac{c_\infty}{e_q - 1} \left((P_i^{n+1})^2 - (P_i^n)^2 \right) \right] \leq 0 \quad (4.52)$$

which implies, using definition (4.42) that

$$\mathcal{E}_h^{n+1} \leq \mathcal{E}_h^n,$$

i.e., the energy (4.42) decays with time. This also implies the unconditional stability of the sequential splitting scheme. \square

4.5 Von Neumann Analysis of E-OS Scheme

Since the models considered are linear, we can use Fourier analysis to study dissipation and dispersion errors in the sequential splitting scheme. We assume the spatial dependence $[1, 7]$ $V_j^n = \tilde{V}^n e^{ikj\Delta z}$ for all field variables V . Here $i = \sqrt{-1}$ and k is the wave number. The $\tilde{}$ superscript on the field variable V denotes a Fourier transform. From equation (4.23), we obtain

$$\tilde{P}^{n+1} = \frac{2\gamma}{c_\infty(2\tau - \gamma + \Delta t)} \tilde{E}^{n+1} + \frac{2\tau - \gamma - \Delta t}{2\tau - \gamma + \Delta t} \tilde{P}^n. \quad (4.53)$$

Equations (4.22) and (4.21) (assuming $J_s = 0$) give us the relations

$$\tilde{E}^{n+1} = \left(\frac{2\tau - \gamma}{2\tau + \gamma} \right) \tilde{E}^n + \theta \left(\frac{2\tau - \gamma}{2\tau + \gamma} \right) (\tilde{H}^{n+1} + \tilde{H}^n) + \frac{c_\infty \Delta t}{2\tau + \gamma} (\tilde{P}^{n+1} + \tilde{P}^n) \quad (4.54)$$

$$\tilde{H}^{n+1} = \tilde{H}^n + \frac{\theta}{2\tau - \gamma} \left((2\tau + \gamma) \tilde{E}^{n+1} + (2\tau - \gamma) \tilde{E}^n - c_\infty \Delta t (\tilde{P}^{n+1} + \tilde{P}^n) \right), \quad (4.55)$$

where $\gamma = \Delta t(\varepsilon_q - 1)$, and $\theta = \eta_\infty i \sin(\frac{k\Delta z}{2})$.

We rewrite the system of equations (4.53), (4.54), and (4.55) into the form $\tilde{\mathbf{U}}^{n+1} = \mathbf{A} \tilde{\mathbf{U}}^n$, where \mathbf{A} is the amplification matrix for the system. To quantify the **numerical dissipation error**, we plot the maximum complex-time eigenvalue of the characteristic polynomial of the amplification matrix \mathbf{A} . We do this numerically, by choosing the following values for the parameters of the Maxwell-Debye model.

$$\epsilon_\infty = 1 \quad (4.56)$$

$$\epsilon_s = 80.3 \quad (4.57)$$

$$\tau = 8.13 \times 10^{-12} \text{ sec.} \quad (4.58)$$

These are appropriate constants for modeling water and are representative of a large class of Debye type materials [2].

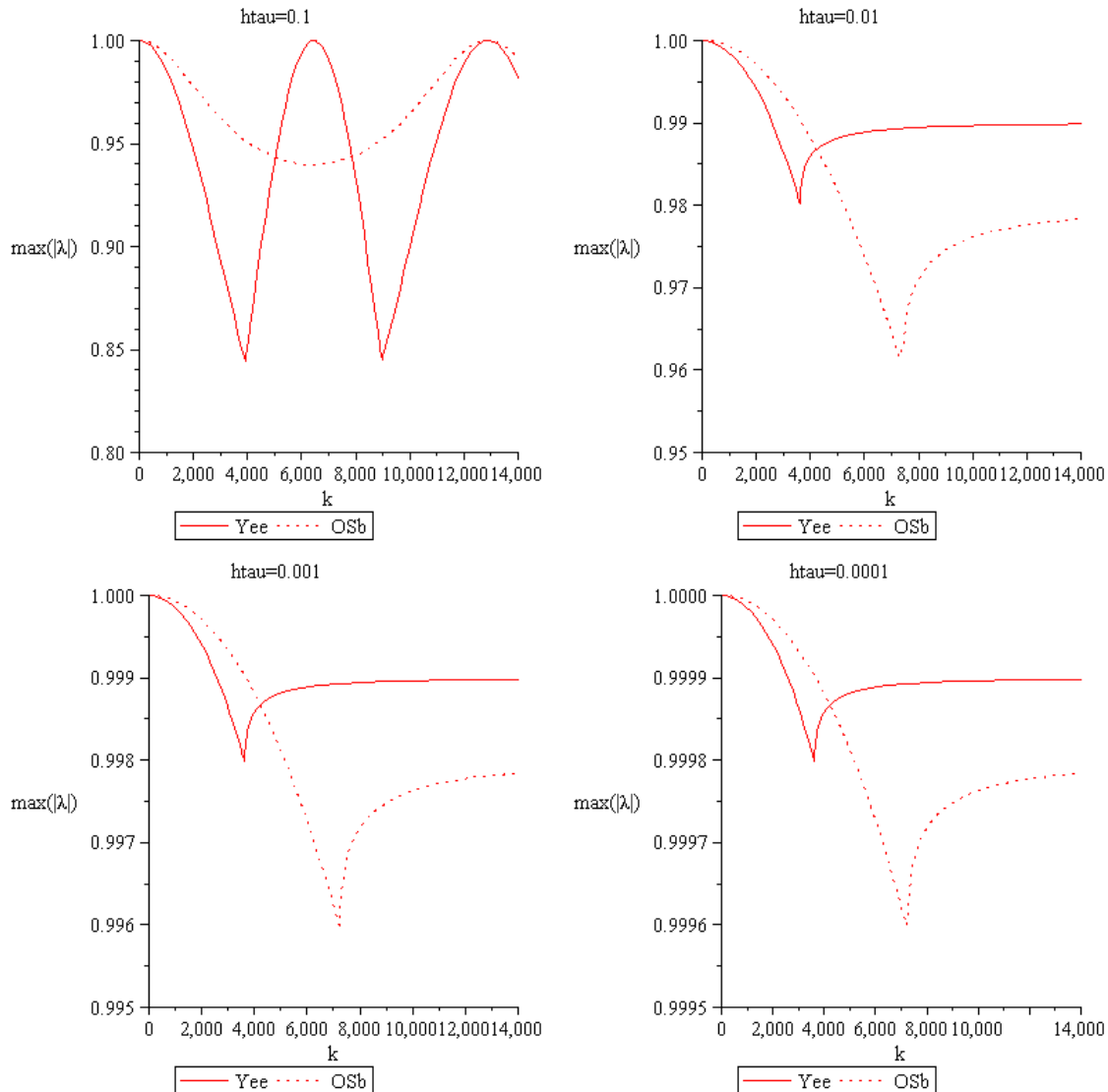
For accuracy, the numerical schemes for Debye media must resolve the smallest time scale, i.e., the relaxation time or the period of the highest frequency component of the electric field. Thus, the parameters

$$(P1) \quad h_\tau = \frac{\Delta t}{\tau}$$

$$(P2) \quad h_\omega = \frac{\Delta t}{2\pi/\omega}$$

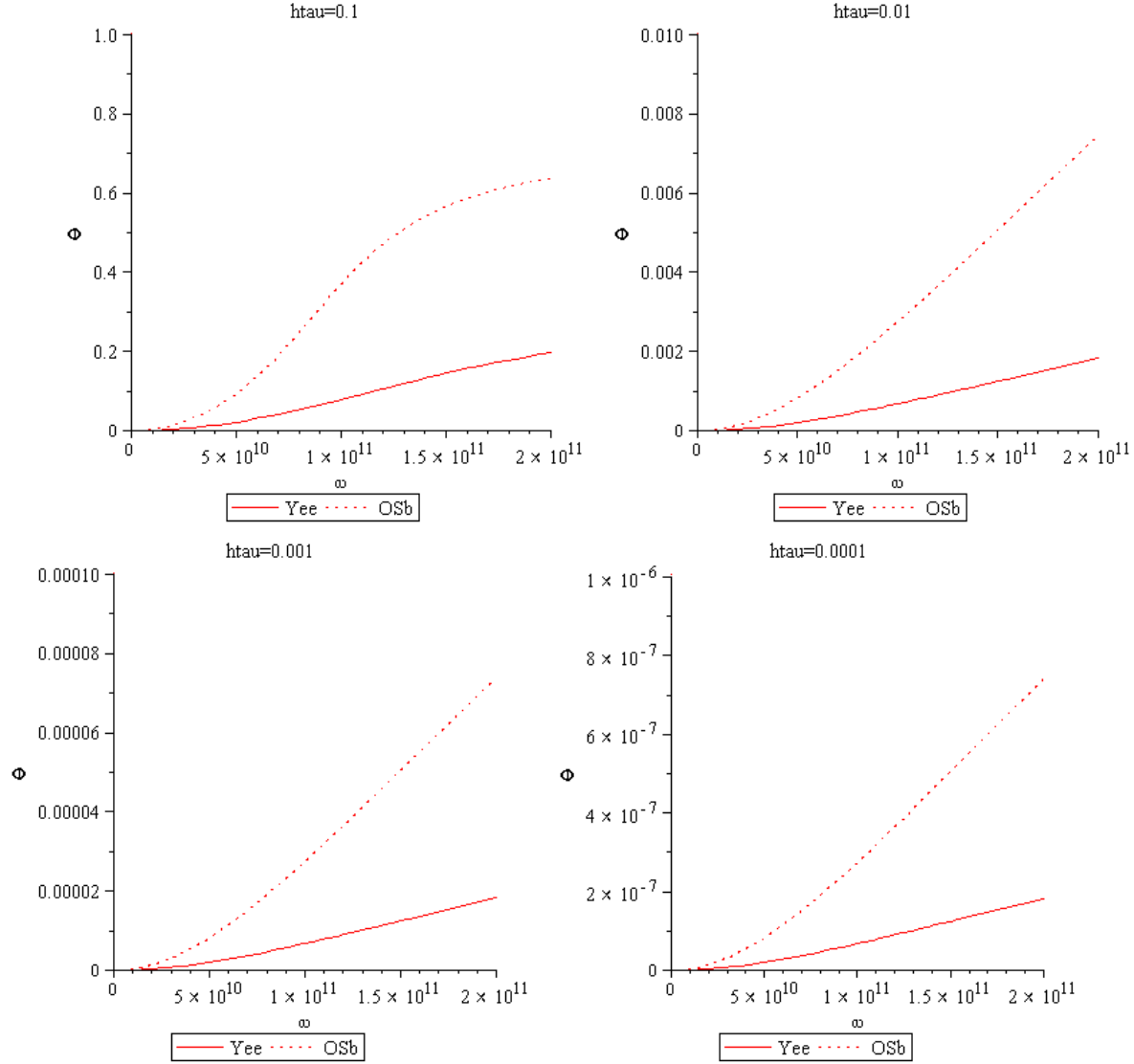
must be sufficiently small. Both η_∞ and h_ω determine the spatial resolution of the wavelength of the electric field. (i.e., points per wavelength). In Figure 5 we compare dissipation error between the sequential operator splitting scheme and the Yee scheme, plotting the modulus of the largest eigenvalue $\max|\lambda|$ of the amplification matrix as a function of k for various values of h_τ .

Figure 5: Dissipation Error



4.6 Dispersion of Equivalent Operator Splitting Scheme

Figure 6: Phase Error and Numerical Dispersion



We next compute the numerical dispersion relation for the scheme **(E-OS)**. The exact dispersion relation for Maxwell-Debye media is

$$k_{ex}(\omega) = \frac{\omega}{c} \sqrt{\frac{\varepsilon_s - i\omega\tau\varepsilon_\infty}{1 - i\omega\tau}}. \quad (4.59)$$

To compute the numerical dispersion relation we assume the spatio-temporal dependence

$$V_j^n = V_0 e^{-i\omega n \Delta t} e^{ijk \Delta z}. \quad (4.60)$$

for all field variables V , with

$$\tilde{V}^n = V_0 e^{-i\omega n \Delta t}, \quad (4.61)$$

This implies the identity

$$(\mathbf{A} - e^{-i\omega\Delta t}\mathbf{I})\mathbf{U}_0 = 0, \quad (4.62)$$

where $\mathbf{U}_0 = [H_0, E_0, P_0]^T$, and \mathbf{I} is the identity matrix. Thus, the matrix $(\mathbf{A} - e^{-i\omega\Delta t}\mathbf{I})$ is singular, and we obtain the numerical dispersion relation for the sequential splitting scheme as

$$\det(\mathbf{A} - e^{-i\omega\Delta t}\mathbf{I}) = 0. \quad (4.63)$$

We define the **phase error** Φ as

$$\Phi(\omega) = \frac{|k(\omega) - k_{ex}(\omega)|}{|k_{ex}(\omega)|}. \quad (4.64)$$

Using the same parameter values as in the dissipation analysis, we plot the phase error for the Yee scheme and the sequential splitting scheme in Figure 6, again for various values of the parameter h_τ .

4.7 Pulse Propagation Experiment

In this section we perform a simulation of the propagation of a 1 nanosecond duration square modulated sine wave with carrier frequency 10GHz normally incident on a Debye medium half space from the air-side [1, 7], using both the Yee scheme, and the sequential operator splitting (**SS-D**) method. This same pulse shown in Figure 7 was used as the input source term for implementations of both the Yee scheme and the operator splitting scheme. In Figure 8 we draw a comparison for different values of h_τ . We simulate the Yee scheme for $h_\tau = 0.001$. The plot in Figure 8 shows the value of the electric field E taken at a sampling point of 0.15m inside the Debye medium.

Figure 7: Source

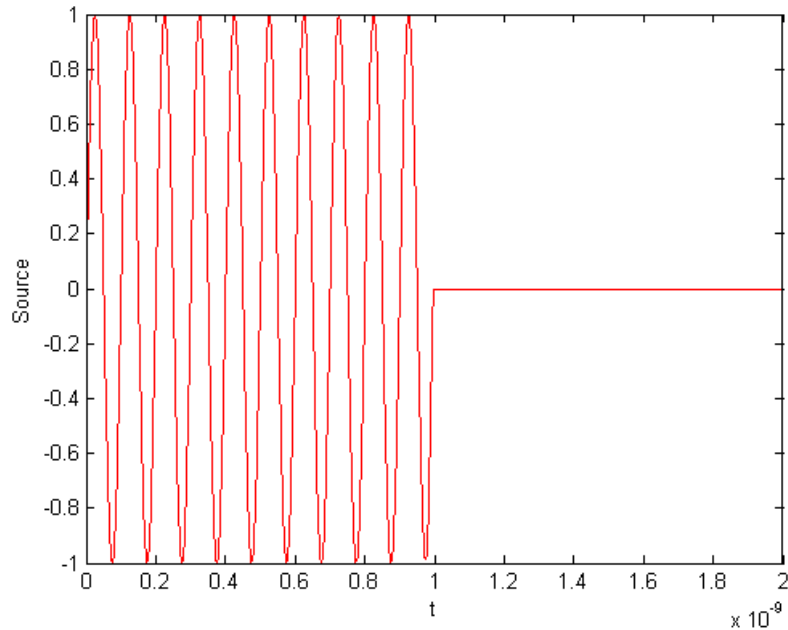
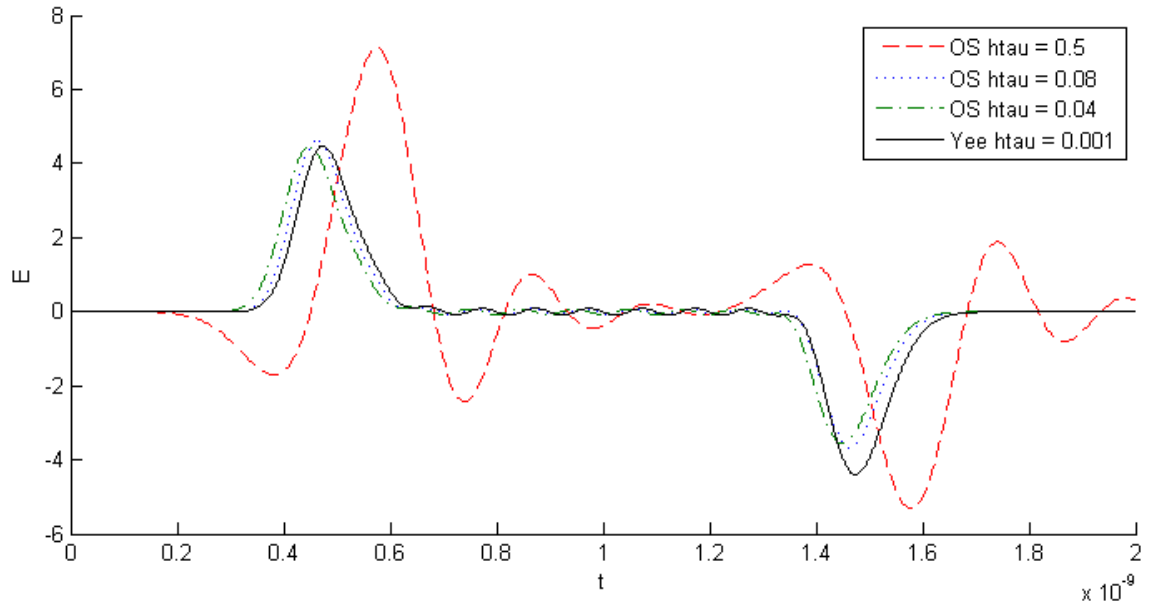
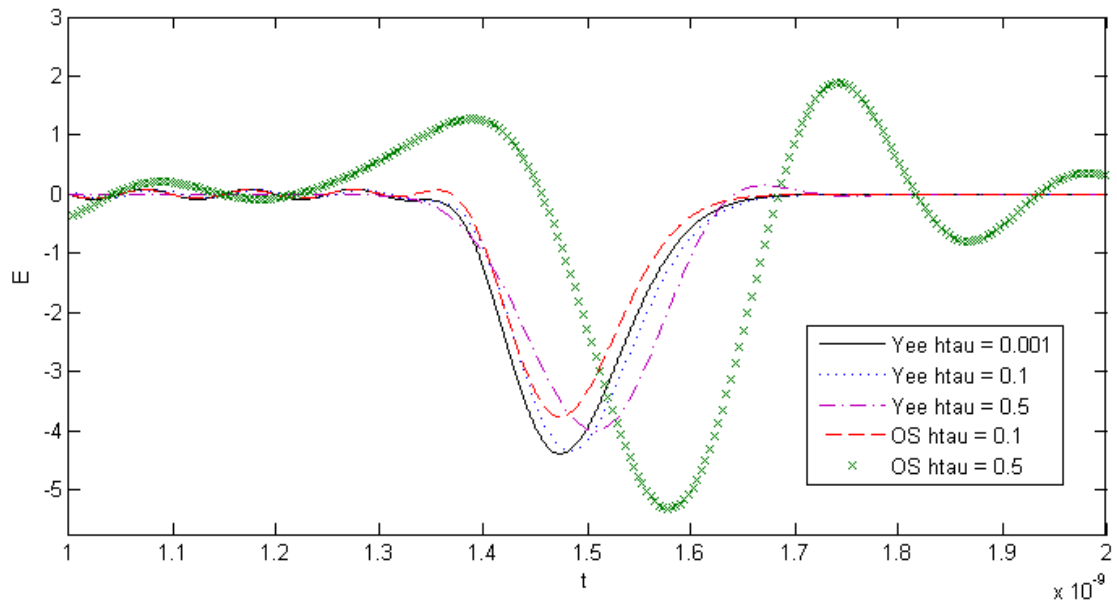


Figure 8: Comparison of Yee and Operator Splitting Schemes



In Figure 9 we compare the Yee and operator splitting scheme for different h_τ .

Figure 9: Convergence of Sequential Operator Splitting Method w.r.t h_τ



5 Conclusion

We have constructed an unconditionally stable numerical scheme for electromagnetic wave propagation in a Debye dispersive medium using operator splitting techniques in one dimension. This method is first order accurate in time and second order accurate in space. Numerical dispersion and dissipation errors were examined and compared to the Yee scheme. The dissipation and phase error plots indicate that these errors are comparable in both schemes for small values of the parameter h_τ .

Planned future work includes extension to three dimensions and a complete analysis of the scheme's properties in two and three dimensions. The use of symmetrized splitting [8] in order to obtain an OS scheme with second order accuracy in time is also under consideration.

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