AN FDTD ALGORITHM FOR WAVE PROPAGATION IN DISPERSIVE MEDIA USING HIGHER-ORDER SCHEMES

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Abstract—A fourth-order accurate in space and second-order accurate in time, Finite-Difference Time-Domain (FDTD) scheme for wave propagation in lossy dispersive media is presented. The formulation of Maxwell’s equations is fully described and an elaborate study of the stability and dispersion properties of the resulting algorithm is conducted. The efficiency of the proposed FDTD(2,4) technique compared to its conventional FDTD(2,2) counterpart is demonstrated through numerical results.

1 Introduction

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1. INTRODUCTION

The Finite Difference Time Domain (FDTD) method [1, 2] has prevailed in the computational electromagnetics area as an accurate numerical technique for the direct integration of Maxwell’s equations. Its evolution has ensued from several technological developments, resulting in the emergence of various algorithms that extend the method’s implementation to various modern applications. A major group of such problems involves pulse propagation inside dispersive materials. Representative examples are the simulation of light propagation in optical devices, soil modeling in ground penetrating radar (GPR) problems [3], and study of potential effects of human tissue exposure to electromagnetic radiation.

The techniques that render the FDTD method suitable for dispersive media modeling are grounded on an appropriate formulation of either the equation of motion of charged particles, or the local constitutive relation connecting the dielectric displacement to the electric field. In the former occasion a differential equation, which describes the electric field dependence on the polarization current density, is derived and discretized via regular differencing rules [4, 5]. For the latter case three popular approaches have been presented. The Auxiliary Differential Equation (ADE) [6] technique translates the frequency-dependent constitutive relation in the time domain, by inverse Fourier transform, leading to an ordinary differential equation. The $Z$-transform based method [7] concludes in a similar differential equation, assuming the complex permittivity in the $Z$-domain to be a transfer function. Finally, in the Recursive Convolution (RC) [1] formulation the convolution integral corresponding to the time domain constitutive relation is approximated by a discrete summation which is then properly calculated using a recursive procedure.

The accuracy of the aforementioned efforts for expanding the FDTD method to frequency dependent materials is controlled by the choice of the spatial increment. Specifically, Yee’s scheme is characterized by numerical dispersion errors which accumulate in time and contaminate the solution. This side-effect is limited by using very fine discretization. Considering the fact that FDTD techniques for dispersive media introduce auxiliary variables or store field values from previous time steps, the fine mesh is translated into excessive memory demands. Furthermore, the achievement of high frequency resolution requires elongated simulations. An obvious way to restrict the memory needs and total computational times is the use of higher-order schemes [8–12]. A fourth-order accurate in time and space FDTD approach for propagation in collisionless plasma has been presented in [13].
the accuracy and memory savings achieved, the proposed method is restricted to lossless dispersive media. Recently, in [14], a novel higher-order method for modeling lossy media has been presented.

In this paper, a staggered fourth-order accurate in space and second-order accurate in time FDTD scheme for the simulation of lossy dispersive materials is proposed. The media considered are second- and Nth-order Lorentz, first- and Mth-order Debye, and second-order Drude. The algorithm is based on the ADE technique [6], while a material-independent perfectly matched layer (PML) [15] is utilized for the reflectionless truncation of the computational domain. The stability and numerical dispersion characteristics of the proposed technique, examined for the (2,2) case in [16], are investigated through the derivation of an appropriate stability criterion as well as a dispersion relation for each material.

## 2. HIGHER-ORDER FDTD SCHEMES FOR DISPERSIVE MEDIA

The key premise of the proposed FDTD(2,4) method is the discretization of the spatial and temporal derivatives using fourth-order and second-order approximations, respectively. In order to present a more compact methodology for wave propagation in dispersive media, temporal central finite difference- ($\delta_t$, $\delta_{2t}$, $\delta_{2t}^2$), central average- ($\mu_t$, $\mu_{2t}$) and central spatial-operators $\delta_{\beta}$ are defined in Tables 1 and 2. In the context of this paper the spatial derivative $\partial/\partial \beta$ is substituted by the fourth-order spatial operator

$$
\frac{1}{\Delta \beta} \delta_{\beta} F_m = \frac{1}{24 \Delta \beta} \left( F_{m - \frac{3}{2}} - 27 F_{m - \frac{1}{2}} + 27 F_{m + \frac{1}{2}} - F_{m + \frac{3}{2}} \right)
$$

(1)

where the index $m$ corresponds to $\beta$ coordinate, unless stated otherwise.

**Table 1. Temporal approximations.**

<table>
<thead>
<tr>
<th></th>
<th>Time-domain</th>
<th>Z-domain</th>
<th>$\omega$-domain</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\delta_t F^n$</td>
<td>$F^{n+1/2} - F^{n-1/2}$</td>
<td>$Z^{1/2} - Z^{-1/2}$</td>
<td>$2j \sin(\omega \Delta t / 2)$</td>
</tr>
<tr>
<td>$\delta_{2t} F^n$</td>
<td>$\frac{1}{2} \left( F^{n+1} - F^{n-1} \right)$</td>
<td>$\frac{1}{2} \left( Z - Z^{-1} \right)$</td>
<td>$j \sin(\omega \Delta t)$</td>
</tr>
<tr>
<td>$\mu_t F^n$</td>
<td>$\frac{1}{2} \left( F^{n+1/2} + F^{n-1/2} \right)$</td>
<td>$\frac{1}{2} \left( Z^{1/2} + Z^{-1/2} \right)$</td>
<td>$\cos(\omega \Delta t / 2)$</td>
</tr>
<tr>
<td>$\mu_{2t} F^n$</td>
<td>$\frac{1}{2} \left( F^{n+1} + F^{n-1} \right)$</td>
<td>$\frac{1}{2} \left( Z + Z^{-1} \right)$</td>
<td>$\cos(\omega \Delta t)$</td>
</tr>
<tr>
<td>$\delta_t^2 F^n \equiv \delta_t(\delta_t F^n)$</td>
<td>$F^{n+1} - 2F^n + F^{n-1}$</td>
<td>$Z + Z^{-1} - 2$</td>
<td>$-4 \sin^2(\omega \Delta t / 2)$</td>
</tr>
</tbody>
</table>
Table 2. Spatial approximations.

<table>
<thead>
<tr>
<th>Order</th>
<th>Formula</th>
<th>Eigenvalues</th>
</tr>
</thead>
<tbody>
<tr>
<td>2nd-order</td>
<td>$F_{m+1/2} - F_{m-1/2}$</td>
<td>$2j \sin(k_{num,\beta} \Delta \beta/2)$</td>
</tr>
<tr>
<td>4th-order</td>
<td>$-\frac{1}{24}(F_{m+3/2} - F_{m-3/2}) + \frac{9}{8}(F_{m+1/2} - F_{m-1/2})$</td>
<td>$2j \left[ \frac{9}{8} \sin(k_{num,\beta} \Delta \beta/2) - \frac{1}{24} \sin(3k_{num,\beta} \Delta \beta/2) \right]$</td>
</tr>
<tr>
<td>6th-order</td>
<td>$\frac{3}{640}(F_{m+5/2} - F_{m-5/2})$</td>
<td>$2j \left[ \frac{75}{64} \sin(k_{num,\beta} \Delta \beta/2) - \frac{25}{384} \sin(3k_{num,\beta} \Delta \beta/2) + \frac{3}{640} \sin(5k_{num,\beta} \Delta \beta/2) \right]$</td>
</tr>
</tbody>
</table>

The simulation of dispersive materials is founded on the ADE technique. Wave propagation inside the medium is fully described by the two Maxwell’s laws, which are discretized using the FDTD(2,4) scheme, and the frequency-dependent constitutive relation $D(r, \omega) = \epsilon(\omega)E(r, \omega)$, where $\epsilon(\omega)$ is the complex permittivity defining the material’s dispersion properties. Taking the inverse Fourier transform of the previous constitutive relation, an ordinary differential equation is derived, which is then discretized utilizing a central differencing scheme in time. Assuming an $N$th-order dispersion, the process, which has been just described, results in

$$E^{n+1} = f \left( E^n, \ldots, E^{n-N+1}, D^{n+1}, D^n, \ldots, D^{n-N+1} \right)$$

(2)

The two discretized Maxwell’s equations along with (2) constitute the overall computation model.

2.1. Debye Medium

In the case of the first-order Debye dispersion, the complex permittivity function is

$$\epsilon(\omega) = \epsilon_{\infty} + \frac{\epsilon_s - \epsilon_{\infty}}{1 + j\omega\tau}$$

(3)

where $\epsilon_s = \epsilon(0)$, $\epsilon_{\infty} = \epsilon(\infty)$ and $\tau$ denotes the relaxation time constant. Applying the inverse Fourier transform, considering an $e^{j\omega t}$ dependence, results in the following differential equation

$$D + \tau \frac{\partial D}{\partial t} = \epsilon_s E + \epsilon_{\infty} \tau \frac{\partial E}{\partial t}$$

(4)
High-order FDTD for dispersive media

which is discretized utilizing the proper temporal and averaging operators of Table 1

\[
\left( \mu_t + \tau \frac{\delta t}{\Delta t} \right) D^n = \left( \epsilon_s \mu_t + \epsilon_\infty \tau \frac{\delta t}{\Delta t} \right) E^n
\]  

(5)

and solved for \( E^{n+1} \) in terms of known values of the electric field and the dielectric displacement as

\[
E^{n+1} = \frac{(2\epsilon_\infty \tau - \epsilon_s \Delta t)E^n + (\Delta t - 2\tau)D^n + (\Delta t + 2\tau)D^{n+1}}{2\epsilon_\infty \tau + \epsilon_s \Delta t}
\]  

(6)

In the case of a general \( M \)-th order Debye material, the complex permittivity is defined as

\[
\epsilon(\omega) = \epsilon_\infty + \sum_{n=1}^{M} \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega \tau_n}
\]  

(7)

where \( \tau_n \) is the relaxation time constant corresponding to the \( n \)-th pole. The previous methodology is extended by introducing \( M \) additional electric field polarization terms \( P_\eta \) as

\[
D = \epsilon_\infty E + \sum_{\eta=1}^{M} P_\eta
\]  

(8)

\[
P_\eta = \frac{\epsilon_s - \epsilon_\infty}{1 + j\omega \tau_n} E
\]  

(9)

leading to the following differential equation for the \( \eta \)-th pole

\[
P_\eta + \tau_\eta \frac{\partial P_\eta}{\partial t} = (\epsilon_s - \epsilon_\infty)E, \quad \eta = 1, 2, \ldots, M
\]  

(10)

The discretized form of (10) is

\[
(\mu_t + \tau_\eta \delta_t) P_\eta^n = (\epsilon_s - \epsilon_\infty) \mu_tE^n
\]  

(11)

yielding, along with (8), the final expression for computing the electric field

\[
E^{n+1} = \frac{1}{c_4} \left[ D^{n+1} - \sum_{\eta=1}^{M} \frac{1}{c_1^{\eta}} \left( c_2^{\eta} P_\eta^n + c_3^{\eta} E^n \right) \right]
\]  

(12)

where the constants \( c_1^{\eta}, c_2^{\eta}, c_3^{\eta} \) and \( c_4 \) are defined as

\[
c_1^{\eta} = 2\tau_\eta + \Delta t, \quad c_2^{\eta} = 2\tau_\eta - \Delta t, \quad c_3^{\eta} = (\epsilon_s - \epsilon_\infty) \Delta t, \quad c_4 = \epsilon_\infty + \sum_{\eta=1}^{M} \frac{\epsilon_s - \epsilon_\infty}{2\tau_\eta + \Delta t} \Delta t
\]  

(13)
Finally, the summation terms $P_{n+1}^\eta$ are calculated through

$$P_{n+1}^\eta = \frac{1}{c_1^\eta} \left[ c_2^\eta P_n^\eta + c_3^\eta (E^{n+1} + E^n) \right]$$  \hspace{1cm} (14)

### 2.2. Lorentz Medium

The complex permittivity describing a second-order Lorentz-type chromatic dispersion is

$$\epsilon(\omega) = \epsilon_{\infty} + (\epsilon_s - \epsilon_{\infty}) \frac{\omega_0^2}{\omega_0^2 + 2j\omega_0\delta_0 - \omega^2}$$  \hspace{1cm} (15)

where $\epsilon_s = \epsilon(0)$, $\epsilon_{\infty} = \epsilon(\infty)$, $\omega_0$ is the resonant frequency of the medium and $\delta_0$ a damping coefficient. The governing differential equation is

$$\omega_0^2 D + 2\delta_0 \frac{\partial D}{\partial t} + \frac{\partial^2 D}{\partial t^2} = \epsilon_{\infty} \frac{\partial^2 E}{\partial t^2} + 2\delta_0 \epsilon_{\infty} \frac{\partial E}{\partial t} + \omega_0^2 \epsilon_s E$$  \hspace{1cm} (16)

which can be discretized in the same manner as in the Debye medium

$$\left[ \omega_0^2 \mu_2 + \frac{2\delta_0}{\Delta t} \delta t \mu_1 + \frac{\delta_1^2}{(\Delta t)^2} \right] D^n = \left[ \epsilon_{\infty} \frac{\delta_1^2}{(\Delta t)^2} + \frac{2\delta_0 \epsilon_{\infty}}{\Delta t} \delta t \mu_1 + \omega_0^2 \epsilon_s \mu_2 \right] E^n$$  \hspace{1cm} (17)

and solved for $E^{n+1}$ in terms of known $E$ and $D$ values. The resultant expression is that of [6] and is repeated below

$$E^{n+1} = \left\{ \begin{array}{l} D^{n+1} \left[ 2 + 2\delta_0 \Delta t + \omega_0^2 (\Delta t)^2 \right] - 4D^n \\
+ \left[ 2 - 2\delta_0 \Delta t + \omega_0^2 (\Delta t)^2 \right] D^{n-1} \\
- \left[ 2\epsilon_{\infty} - 2\delta_0 \epsilon_{\infty} \Delta t + \epsilon_s \omega_0^2 (\Delta t)^2 \right] E^{n-1} + 4\epsilon_{\infty} E^n \end{array} \right\} / \left\{ 2\epsilon_{\infty} + 2\delta_0 \epsilon_{\infty} \Delta t + \epsilon_s \omega_0^2 (\Delta t)^2 \right\}$$  \hspace{1cm} (18)

For an $N$-th order Lorentz medium with a resonant frequency $\omega_n$ and a damping coefficient $\delta_n$ the macroscopic permittivity function $\epsilon(\omega)$ is

$$\epsilon(\omega) = \epsilon_{\infty} + (\epsilon_s - \epsilon_{\infty}) \sum_{n=1}^{N} \frac{G_n \omega_n^2}{\omega_n^2 + 2j\omega_0 \delta_n - \omega^2}$$  \hspace{1cm} (19)

where $\sum_{n=1}^{N} G_n = 1$. The dispersion properties of the material are described, similarly to the $M$-th order Debye model, by the following
\[ D = \epsilon_{\infty} E + \sum_{\eta=1}^{N} P_\eta \]  
\[ \omega^2_\eta P_\eta + 2\delta_\eta \frac{\partial P_\eta}{\partial t} + \frac{\partial^2 P_\eta}{\partial t^2} = G_\eta (\epsilon_s - \epsilon_{\infty}) \omega^2_\eta E, \quad \eta = 1, 2, \ldots, N \]  
Equation (20b) is written in difference terms
\[ \left[ \omega^2_\eta \mu_2 t + \frac{2\delta_\eta}{\Delta t} \delta_t \mu_t + \frac{\delta^2_t}{(\Delta t)^2} \right] P^n_\eta = G_\eta (\epsilon_s - \epsilon_{\infty}) \omega^2_\eta \mu_2 E^n \]  
leading, in combination with (20a), to the evaluation of the electric field \( E^{n+1} \)
\[ E^{n+1} = \frac{1}{c_4} \left[ D^{n+1} - \sum_{\eta=1}^{N} \frac{1}{c_1^\eta} \left( 4P^n_\eta - c_2^\eta P_\eta^{n-1} + c_3^\eta E^{n-1} \right) \right] \]  
where the constants \( c_1^\eta, c_2^\eta, c_3^\eta \) and \( c_4 \) are defined as
\[ c_1^\eta = \omega^2_\eta (\Delta t)^2 + 2\delta_\eta \Delta t + 2, \quad c_2^\eta = \omega^2_\eta (\Delta t)^2 - 2\delta_\eta \Delta t + 2, \]  
\[ c_3^\eta = G_\eta (\epsilon_s - \epsilon_{\infty}) \omega^2_\eta (\Delta t)^2, \quad c_4 = \epsilon_{\infty} + \sum_{\eta=1}^{N} \frac{c_3^\eta}{c_1^\eta} \]  
and the dielectric displacement \( D^{n+1} \) is calculated from Ampére’s law. The index \( \eta \) is used to denote the respective resonant frequency. After updating \( E^{n+1} \), the values \( P_\eta^{n+1} \) are computed by (21) which is formulated as
\[ P_\eta^{n+1} = \frac{1}{c_1^\eta} \left[ 4P_\eta^n - c_2^\eta P_\eta^{n-1} + c_3^\eta (E^{n+1} + E^{n-1}) \right] \]  
2.3. Drude Medium
The Drude model, related to the cold plasma, is described by the following permittivity function
\[ \epsilon(\omega) = \epsilon_0 \left[ 1 + \frac{\omega_p^2}{\omega(j\nu_c - \omega)} \right] \]
where $\omega_p$ is the radian plasma frequency and $\nu_c$ is the collision frequency. The governing differential equation is

$$\nu_c \frac{\partial D}{\partial t} + \frac{\partial^2 D}{\partial t^2} = \epsilon_0 \left( \frac{\omega_p^2 E}{\epsilon_0} + \nu_c \frac{\partial E}{\partial t} + \frac{\partial^2 E}{\partial t^2} \right)$$  \hspace{1cm} (26)

which is written in difference notation as

$$\left[ \nu_c \frac{\delta^2}{\Delta t^2} + \frac{\delta_t^2}{(\Delta t)^2} \right] D^n = \epsilon_0 \left[ \frac{\omega_p^2 \mu^2}{\epsilon_0} \frac{\delta^2}{\Delta t^2} + \frac{\delta_t^2}{(\Delta t)^2} \right] E^n$$  \hspace{1cm} (27)

and solved for $E^{n+1}$ to obtain

$$E^{n+1} = \frac{1}{\epsilon_0} \left\{ 4\epsilon_\infty E^n - \epsilon_0 \left[ \frac{\omega_p^2 (\Delta t)^2}{\epsilon_0} - \nu_c (\Delta t) + 2 \right] E^{n-1} + (2 + \nu_c (\Delta t)) D^{n+1} - 4D^n + (2 - \nu_c (\Delta t)) D^{n-1} \right\} / \left[ \frac{\omega_p^2 (\Delta t)^2}{\epsilon_0} + \nu_c (\Delta t) + 2 \right]$$  \hspace{1cm} (28)

3. STABILITY ANALYSIS

Among the principal properties of the FDTD method, inherent in explicit differential equation solvers, is the conditional stability. In the conventional Yee’s scheme the unbounded growth of errors is eluded by the proper choice of the time step size dictated by the Courant condition. The stability characteristics of the proposed higher-order algorithm are investigated using the methodology presented in [17], which combines the von Neumann method with the Routh-Hurwitz criterion. It is presumed that the error present in the computation of any field quantity $F$ is described by a single term of a Fourier series expansion

$$F^n = F_0 Z^n e^{j \sum_{\beta=x,y,z} k_{num,\beta} m \Delta \beta}$$  \hspace{1cm} (29)

where the complex variable $Z$ corresponds to the growth factor of the error. Under this assumption, the temporal differencing and averaging operators as well as the spatial differencing operators are evaluated as shown in Tables 1 and 2.

The time-dependent wave equation in a source-free homogeneous dispersive medium is

$$\mu \frac{\partial^2 D}{\partial t^2} - \nabla^2 E = 0$$  \hspace{1cm} (30)

and approximated by

$$\mu \frac{\delta^2}{(\Delta t)^2} D^n - \sum_{\beta=x,y,z} \frac{\delta^2}{(\Delta \beta)^2} E^n = 0$$  \hspace{1cm} (31)
where $\delta_\beta$, ($\beta = x, y, z$) denotes the central spatial difference operator of arbitrary order with respect to the coordinate indicated by the subscript. Solutions of the form (29) are substituted in (31) leading to a polynomial in $Z$. The stability of the finite difference scheme is assured if the roots of this characteristic polynomial are located inside or on the unit circle in the $Z$-plane, namely $|Z| \leq 1$. The bilinear transformation

$$Z = \frac{r + 1}{r - 1}$$

is then applied to the stability polynomial. In this way, the exterior of the unit circle in the $Z$-plane is mapped on the right-half of the $r$-plane. In order to examine whether the root of the polynomial with respect to $r$ are nonnegative, the Routh table is created. If the values of all the elements in the first column are positive or zero, the algorithm is stable. The enforcement of the stability constraint regarding the specified entries of the Routh table results in certain inequalities relating the parameters of the FDTD scheme.

Following the procedure which has just been described, (31) is formulated, with the use of Tables 1 and 2, as

$$(Z - 1)^2 D_0 + 4Z\epsilon_\infty \nu^2 E_0 = 0$$

where

$$\nu^2 = (c_\infty \Delta t)^2 \sum_{\beta=x,y,z} \frac{1}{(\Delta \beta)^2} \left[ \frac{9}{8} \sin \left( k_{\text{num},\beta} \frac{\Delta \beta}{2} \right) - \frac{1}{24} \sin \left( k_{\text{num},\beta} \frac{3\Delta \beta}{2} \right) \right]^2$$

for fourth-order accuracy in space and $c_\infty = 1/\sqrt{\mu\epsilon_\infty}$. A formula similar to (34) can be derived in a straightforward manner for any spatial approximation order. The spatial discretization operators are shown in Table 2 for the case of second- and sixth-order.

Next, the stability properties of the FDTD(2,4) scheme for the three aforementioned dispersive media will be examined. In the case of the Drude model the methodology will be presented in detail, while for the Debye and Lorentz models only the final results will be provided.

The constitutive relation in the $Z$-domain for the Drude model is

$$\epsilon_0 \left( \left[ \frac{\omega_p^2}{2} + \frac{\nu_c}{\Delta t} + \frac{1}{(\Delta t)^2} \right] Z^2 - \frac{2}{(\Delta t)^2} Z + \frac{\omega_p^2}{2} - \frac{\nu_c}{\Delta t} \right) E_0 =$$

$$(Z - 1)^2 D_0 + 4Z\epsilon_\infty \nu^2 E_0$$

and

$$\epsilon_0 \left( \left[ \frac{\omega_p^2}{2} + \frac{\nu_c}{\Delta t} + \frac{1}{(\Delta t)^2} \right] Z^2 - \frac{2}{(\Delta t)^2} Z + \frac{\omega_p^2}{2} - \frac{\nu_c}{\Delta t} \right) E_0$$

for fourth-order accuracy in space and $c_\infty = 1/\sqrt{\mu\epsilon_\infty}$. A formula similar to (34) can be derived in a straightforward manner for any spatial approximation order. The spatial discretization operators are shown in Table 2 for the case of second- and sixth-order.
Solving (33) for $D_0$ results in

$$D_0 = -\frac{4Z\epsilon_0 \nu^2}{(Z-1)^2} E_0$$

Substituting in (35) the characteristic stability polynomial is derived

$$S(Z) = \left[\frac{2}{(\Delta t)^2} + \frac{\nu_c}{\Delta t} + \omega_p^2\right] Z^4 + \left[\frac{8(1-\nu^2)}{(\Delta t)^2} - \frac{2\nu_c(1-2\nu^2)}{\Delta t} - 2\omega_p^2\right] Z^3$$

$$+ \left[\frac{12}{(\Delta t)^2} + \frac{16\nu^2}{(\Delta t)^2}\right] Z^2 + \left[\frac{8(1-\nu^2)}{(\Delta t)^2} - \frac{2\nu_c(1-2\nu^2)}{\Delta t} - 2\omega_p^2\right] Z$$

$$+ \frac{2}{(\Delta t)^2} - \frac{\nu_c}{\Delta t} + \omega_p^2$$

After applying the bilinear transformation, we obtain

$$S(r) = \frac{2\nu^2 \nu_c}{\Delta t} r^3 + \left[\omega_p^2 + \frac{4\nu^2}{(\Delta t)^2}\right] r^2 + \frac{2\nu_c}{\Delta t} (1-\nu^2) + \omega_p^2 + \frac{4}{(\Delta t)^2} - \frac{4\nu^2}{(\Delta t)^2}$$

and the corresponding Routh table is built

| \frac{2\nu^2 \nu_c}{\Delta t} | \frac{2\nu_c}{\Delta t} (1-\nu^2) | \omega_p^2 + \frac{4\nu^2}{(\Delta t)^2} | \omega_p^2 + \frac{4}{(\Delta t)^2} - \frac{4\nu^2}{(\Delta t)^2} | c_3 | c_5 \\
| \omega_p^2 + \frac{4\nu^2}{(\Delta t)^2} | \omega_p^2 + \frac{4}{(\Delta t)^2} - \frac{4\nu^2}{(\Delta t)^2} | c_3 | 0 |

$$c_3 = \frac{2\omega_p^2 \nu_c}{\Delta t} \frac{1 - 2\nu^2}{\omega_p^2 + \frac{4\nu^2}{(\Delta t)^2}}, \quad c_5 = \omega_p^2 + \frac{4(1-\nu^2)}{(\Delta t)^2}$$

Enforcing the entries of the first column to be nonnegative we get

$$\nu^2 \leq 1/2$$

which is translated in the same stability condition as for the Lorentz case, provided below.
Analogously, using the von Neumann method coupled with the Routh-Hurwitz criterion for the Debye-type dispersion the following restraining inequalities are derived
\[ \tau \geq 0, \quad \epsilon_s \geq \epsilon_\infty, \quad \nu^2 \leq 1 \] (41)
the last of which leads to the stability constraint
\[ \Delta t \leq \frac{6}{7} \frac{\sqrt{\mu \epsilon_\infty}}{\tau} \left[ \sum_{\beta=x,y,z} \frac{1}{(\Delta \beta)^2} \right]^{1/2} \] (42)
Similarly, the inequalities for the Lorentz medium are
\[ \nu^2 \leq 1/2, \quad \delta_0 \geq 0, \quad \epsilon_s \geq \epsilon_\infty \] (43)
and the final stability criterion
\[ \Delta t \leq \frac{6}{7} \frac{\sqrt{2 \mu \epsilon_\infty}}{\sqrt{\sum_{\beta=x,y,z} (\Delta \beta)^2}} \] (44)
Numerical simulations have proven that the previous stability conditions are also valid for the general \( N \)th-order Lorentz and \( M \)th-order Debye media.

4. DISPERSION RELATION

4.1. Continuous Dispersion
To determine the dispersion relation in a frequency-dependent medium, harmonic plane wave solutions of the form
\[ F = F_0 \exp[j(\omega t - \gamma \cdot r)] \] (45)
are considered, where \( F \) represents the electric or magnetic field, \( \gamma \) is the propagation vector, \( r \) is the position, and \( t \) the time. Therefore, Maxwell’s equations can be written as
\[ \omega \mu_0 H_0 = \gamma \times E_0 \] (46a)
\[ \omega \epsilon(\omega) E_0 = -\gamma \times H_0 \] (46b)
For isotropic materials, the continuous dispersion relation is
\[ \mu_0 \epsilon(\omega) \omega^2 = \gamma \cdot \gamma \] (47)
It is noted that $\gamma$ is generally a complex vector written as $|\gamma| = \alpha + jk$, where $\alpha$ is the attenuation constant and $k$ is the phase constant. The previous dispersion expression results in

$$k = \frac{\omega}{c_0} \text{Re} \left\{ \frac{\sqrt{\varepsilon(\omega)}}{\varepsilon_0} \right\}$$ (48)

where $c_0 = 1/\sqrt{\varepsilon_0\mu_0}$ is the velocity of light in free space.

4.2. Numerical Dispersion

In order to derive the numerical dispersion relation, the following discrete solution is assumed

$$F^n(I, J, K) = F_0 \exp[j(n\omega\Delta t + Ik_{\text{num},x}\Delta x + Jk_{\text{num},y}\Delta y + Kk_{\text{num},z}\Delta z)]$$ (49)

where indexes $I, J, K$ denote the position of the nodes in the mesh, $\Delta \beta$ ($\beta = x, y, z$) are the sizes of the discretization cell, and $k_{\text{num},\beta}$ ($\beta = x, y, z$) the wavenumbers of the discrete modes in the $\beta$-direction. Similarly to the continuous case, we replace in Maxwell’s equations $\partial/\partial t$ with $j\omega_{\text{num}}$ and $\nabla$ with $-jk_{\text{num}}$, where $\omega_{\text{num}} = \frac{2}{\Delta t} \sin(\omega\Delta t/2)$. Given $\omega_{\text{num}}$ and $k_{\text{num}}$, Maxwell’s equations can be written in discrete form as

$$\omega_{\text{num}}\mu_0 H_0 = k_{\text{num}} \times E_0$$

$$\omega_{\text{num}}\varepsilon_{\text{num}}(\omega_{\text{num}}) E_0 = -k_{\text{num}} \times H_0$$

where $\varepsilon_{\text{num}}$ is the discrete permittivity function defined below. The numerical wavenumber $k_{\text{num}}$ derived for the second-order spatial approximation is

$$k_{\text{num}} = \sum_{\beta=x,y,z} \frac{2}{\Delta \beta} \sin\left(\frac{k_{\text{num},\beta}\Delta \beta}{2}\right) a_\beta$$ (51)

and for the fourth-order spatial approximation

$$k_{\text{num}} = \sum_{\beta=x,y,z} \frac{2}{\Delta \beta} \left[ \frac{9}{8} \left(\frac{k_{\text{num},\beta}\Delta \beta}{2}\right)^2 - \frac{1}{24} \sin\left(\frac{3k_{\text{num},\beta}\Delta \beta}{2}\right) \right] a_\beta$$ (52)

where $a_\beta$ is the unit vector in $\beta$-direction (see Table 2). The previous definitions can be extended to any order of spatial approximation. The central operator of $N$-order ($N$: even number) has the general form

$$\delta_\beta F_m = \sum_{j=1}^{N-1} c_j^N (F_{m+j/2} - F_{m-j/2})$$ (53)
with the coefficients $c_j$ calculated through Taylor series expansions and given in a closed form [18] by

$$c_j^N = \frac{(-1)^{\frac{j}{2}}\frac{1}{2}}{(N-1-j)!!(N-1+j)!!} \left[\frac{(N-1)!!}{2}\right]^2 \sum_{j=1}^{N-1} c_j^N \sin \left(\frac{jk_{num,\beta}\Delta\beta}{2}\right) a_\beta$$

where

$$n!! = \begin{cases} n \cdot (n - 2) \ldots 5 \cdot 3 \cdot 1, & n > 0, \text{ odd} \\ n \cdot (n - 2) \ldots 6 \cdot 4 \cdot 2, & n > 0, \text{ even} \\ 1, & n = -1, 0 \end{cases}$$

Applying the previous formula, the coefficients $c_2^1 = 1$ for Yee’s scheme, $c_4^1 = 9/8$ and $c_4^3 = -1/24$ for Fang’s fourth-order scheme, and $c_6^1 = 75/64$, $c_6^3 = -25/384$, $c_6^5 = 3/640$ for a sixth-order scheme are yielded. It can be easily proven that the numerical wavenumber for the $N$th-order accurate scheme is

$$k_{num} = \sum_{\beta=x,y,z} \frac{2}{\Delta\beta} \sum_{j=1(j \text{ odd})}^{N-1} c_j^N \sin \left(\frac{jk_{num,\beta}\Delta\beta}{2}\right) a_\beta$$

The numerical wavenumber $k_{num}$ is defined as

$$k_{num} = k_{num}(\sin \theta \cos \phi a_x + \sin \theta \sin \phi a_y + \cos \theta a_z)$$

The discrete counterpart of the continuous permittivity function, called numerical permittivity, is defined as the ratio of the discrete values of $D$ and $E$, i.e., $\epsilon_{num} = D^n/E^n$. Similar to the continuous dispersion relation the discrete one is

$$\mu_0 \epsilon_{num}(\omega_{num})\omega_{num}^2 = k_{num} \cdot k_{num}$$

Using the discrete form of the constitutive equation and the temporal operators shown in the third column of Table 1, which are derived by setting $Z = \exp(j\omega t\Delta t)$, the discrete expression of the complex permittivity function for the Lorentz medium is defined as

$$\epsilon_{num} = \epsilon_{\infty} + (\epsilon_s - \epsilon_{\infty}) \frac{\omega_{num,0}^2}{\omega_{num,0}^2 + 2\omega_{num}\delta_{num,0,j} - \omega_{num}^2}$$

where $\omega_{num} = \frac{2}{\Delta t} \sin(\omega \Delta t/2)$, $\delta_{num,0} = \delta_0 \cos(\omega \Delta t/2)$, $\omega_{num,0} = \omega_0 \sqrt{\cos(\omega \Delta t)}$. Analogously, for the Debye medium

$$\epsilon_{num} = \epsilon_{\infty} + \frac{\epsilon_s - \epsilon_{\infty}}{1 + j\omega_{num}\tau_{num}}$$
where $\omega_{\text{num}} = \frac{2}{\Delta} \sin(\omega \Delta t/2)$ and $\tau_{\text{num}} = \tau / \cos(\omega \Delta t/2)$.

Finally, for the Drude medium

$$\epsilon_{\text{num}} = \epsilon_0 \left[ 1 + \frac{\omega_{p,\text{num}}}{\omega_{\text{num}}(j\nu_{c,\text{num}} - \omega_{\text{num}})} \right]$$

(60)

where $\omega_{p,\text{num}} = \omega_p \sqrt{\cos(\omega \Delta t)}$, $\omega_{\text{num}} = \frac{2}{\Delta} \sin(\omega \Delta t/2)$, and $\nu_{c,\text{num}} = \nu_c \cos(\omega \Delta t/2)$.

Restricting ourselves to one-dimensional problems, without loss of generality, it is obtained for the FDTD(2,2) case

$$k_{\text{num}} = \frac{2}{\Delta} \sin^{-1} \left( \frac{\Delta}{2} \omega_{\text{num}} \sqrt{\mu_0 \epsilon_{\text{num}}^0} \right)$$

(61)

for the FDTD(2,4)

$$\frac{2}{\Delta} \left[ \frac{9}{8} \sin \left( \frac{k_{\text{num}} \Delta}{2} \right) - \frac{1}{24} \sin \left( \frac{3k_{\text{num}} \Delta}{2} \right) \right] = \omega_{\text{num}} \sqrt{\mu_0 \epsilon_{\text{num}}^0}$$

(62)

and for the FDTD(2,6)

$$\frac{2}{\Delta} \left[ \frac{75}{64} \sin \left( \frac{k_{\text{num}} \Delta}{2} \right) - \frac{25}{384} \sin \left( \frac{3k_{\text{num}} \Delta}{2} \right) + \frac{3}{640} \sin \left( \frac{5k_{\text{num}} \Delta}{2} \right) \right]$$

$$= \omega_{\text{num}} \sqrt{\mu_0 \epsilon_{\text{num}}^0}$$

(63)

Since these are not in a closed form, to calculate the numerical wavenumber, a numerical technique, like Newton’s iteration method, should be used. In all the previous expressions $k_{\text{num}}$ is assumed to be real and if the right side of the equation is complex only the real part is taken into account. The numerical wavenumber in a 2-D or 3-D problem can be calculated similarly through (56) for different values of propagation angles $\theta$ and $\phi$.

To investigate the dispersive features for both second-, fourth- and sixth-order schemes we consider the following example in a second-order Lorentz medium: Let $\epsilon_{\infty} = 2.25 \epsilon_0$, $\epsilon_s = 3 \epsilon_0$, $\omega_0 = 2\pi f_0$, $f_0 = 200$ MHz and $\delta_0 = 0.1 \omega_0$. Fig. 1 shows the normalized phase velocity $c_{\text{num}}/c = k/\text{Re} \{k_{\text{num}}\}$ for the second-order case with $\Delta = 0.005$ m, $Q = 0.6$ and the fourth- and sixth-order with $\Delta = 0.01$ m, $Q = 0.1$ where the Courant number $Q$ is defined as $Q = c_0 \Delta t/\Delta$. The superior performance of the higher-order schemes is evident, even for larger $\Delta$.

5. NUMERICAL RESULTS

The efficiency of the proposed FDTD(2,4) scheme compared to the conventional second-order accurate technique has been extensively
investigated through numerical results. An analytical reference solution has been developed in order to precisely define the potential errors of each method. The two schemes have been tested in one-dimensional wave propagation problems in homogeneous and inhomogeneous geometries involving materials of diverse dispersion types. In all the examined cases, the new algorithm has been found to be superior, achieving higher accuracy in modeling dispersive characteristics for equal spatial discretization, or allowing a less dense lattice to be used, while the same level of accuracy is ensured.

In the first case studied a Lorentz-type medium slab is placed in free space. The resonant frequency of the material is set to \( \omega_0 = 2 \times 10^9 \text{ rad/sec} \), the damping coefficient is equal to \( \delta_0 = 0.1\omega_0 \), whereas \( \epsilon_\infty = 2.25\epsilon_0 \) and \( \epsilon_s = 3\epsilon_0 \). The wideband reflection coefficient at the interface between air and the dispersive dielectric is calculated by the FDTD(2,2) and FDTD(2,4) ADE techniques. The computational domain consists of 2000 cells and the dielectric slab occupies the region from the 700th cell to 750th cell. For the FDTD(2,4) scheme the spatial step size is set to \( \Delta x = 0.005 \text{ m} \), \( Q = 0.1 \) and the total number of time steps \( N_t = 14250 \). Two sets of parameters are selected for the FDTD(2,2) simulations, namely (a) \( \Delta x = 0.005 \text{ m} \), \( Q = 0.95 \) and \( N_t = 1500 \) and (b) \( \Delta x = 0.0025 \text{ m} \), \( Q = 0.95 \), \( N_t = 3000 \) where the number of cells is doubled. The results for the first case are depicted in

**Figure 1.** Normalized phase velocity as a function of frequency.
Figure 2. The reflection coefficient as a function of frequency. Comparison is made between the exact data, FDTD(2,4) and FDTD(2,2) with $\Delta x = 0.005$ m.

Fig. 2, along with the reference solution. It is clearly observed that the FDTD(2,4) scheme is far more accurate obtaining only slight deviations from the exact reflection coefficient function even for frequencies high above the resonant one. Contrarily, its (2,2) counterpart generates significant errors. The reflection coefficient for the latter group of parameters is illustrated in Fig. 3. The graphs corresponding to the two schemes almost coincide introducing minor shifts in the peaks locations compared to the analytical solution. However, it should be reminded that in the FDTD(2,2) case a two times denser grid is utilized.

In the next simulation, the propagation of the modulated Gaussian pulse $f(t) = \exp\{- (t-t_0)^2/T^2 \} \cos(2\pi f_s t)$ where $t_0 = 8 \times 10^{-9}$ sec, $T = 10^{-9}$ sec and $f_s = 600$ MHz, inside a Lorentz-type dispersive medium is explored. The parameters of the material are $\omega_0 = 2\pi \times 10^6$ rad/sec, $\delta_0 = 0.1\omega_0$, $\epsilon_{\infty} = 2.25\epsilon_0$ and $\epsilon_s = 3\epsilon_0$. For the FDTD(2,2) scheme two different uniform grids are considered: (a) $\Delta x = 0.01$ m, $Q = 0.5$ for 5000 time steps and (b) $\Delta x = 0.05$ m, $Q = 0.5$ for 1000 time steps. The respective parameters for the FDTD(2,4) scheme are $\Delta x = 0.05$ m and $Q = 0.1$. In Fig. 4 the time domain electric field located 0.2 m away from the excitation point is illustrated for the three aforementioned cases along with the exact solution. For an easier observation a detail
Figure 3. The reflection coefficient as a function of frequency. Comparison is made between the exact data, FDTD(2,4) $\Delta x = 0.05$ m, and FDTD(2,2) with $\Delta x = 0.0025$ m.

Figure 4. Electric field waveforms of the exact, FDTD(2,4) and FDTD(2,2) with two different grids.
Figure 5. Detail of Fig. 4. Observe that the proposed technique produces an acceptable close to the (2,2) scheme result but with a five-times coarser grid.

of the previous graphs is shown in Fig. 5. It is evident that the higher-order algorithm achieves the same level of accuracy as the FDTD(2,2) with the first set of parameter values, but with a five times coarser grid. In Table 3, the three methods are compared in terms of maximum error and total computational time. It is noted that the proposed higher-order technique is more accurate and computationally efficient.

Finally, the air-slab problem is solved by the FDTD(2,2) and FDTD(2,4) algorithms assuming that the slab is filled with a third-order Debye dispersive material. The characteristic parameters of the three poles are \( \epsilon_s^1 = 3\epsilon_0, \tau_1 = 9 \times 10^{-9} \text{ sec}, \epsilon_s^2 = 2\epsilon_0, \tau_2 = 10^{-10} \text{ sec} \) and \( \epsilon_s^3 = \epsilon_0, \tau_3 = 10^{-6} \text{ sec} \), while the infinite permittivity is set equal to \( 2.25\epsilon_0 \). In both cases, the computational space consists of 2000 cells, the spatial step size is 0.01 m and \( Q = 0.8 \). The electric field function in the time-domain is presented in Fig. 6. It is again obvious that the proposed higher-order scheme accomplishes better accuracy.

Having verified that FDTD(2,4) can be efficiently extended to dispersive materials, it is applied to wave scattering by an infinite height cylinder made of cold plasma placed in air. The computational space consists of \( 200 \times 200 \) cells. The cylinder is excited by a plane wave. The wavefront is assumed to be a modulated Gaussian pulse centered
Table 3. CPU-time and accuracy comparison for second- and fourth-order schemes.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>$\Delta x$</th>
<th>$Q$</th>
<th>$\text{max(}|\text{error}|)$</th>
<th>CPU-time</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDTD(2,2)</td>
<td>0.05 m</td>
<td>0.5</td>
<td>0.120</td>
<td>0.21 sec</td>
</tr>
<tr>
<td>FDTD(2,2)</td>
<td>0.01 m</td>
<td>0.5</td>
<td>0.055</td>
<td>1.89 sec</td>
</tr>
<tr>
<td>FDTD(2,4)</td>
<td>0.05 m</td>
<td>0.1</td>
<td>0.049</td>
<td>1.52 sec</td>
</tr>
</tbody>
</table>

Figure 6. Electric field waveforms of the exact, FDTD(2,4) and FDTD(2,2).

at 20 GHz. The excitation frequency is stable, while for the plasma frequency of the Drude-type material three values have been selected, namely 28.7 GHz, 5.74 GHz, and 0.287 GHz. In Fig. 7, a snapshot of the electric field, at a time instant when the incident wave has already been scattered by the cylinder, is shown. The frequency components of the incident field are all lower than the plasma frequency. In this case, the Drude dielectric material behaves like a waveguide below cutoff frequency. Indeed, the electric field is not allowed to propagate inside the cylinder. In the second case, shown in Fig. 8, there are
Figure 7. Electric field snapshot for $\omega_p = 28.7\text{ GHz}$.

Figure 8. Electric field snapshot for $\omega_p = 5.74\text{ GHz}$. 
some frequency components of the plane wave, located higher than the plasma frequency. Therefore, a slight deformation of the electric field near the cylinder boundaries is observed. Finally, when the plasma frequency is very low compared to the frequencies contained in the incident field, the plasma cylinder resembles air, as demonstrated in Fig. 9. The electric field travels through it without any modification.

6. CONCLUSIONS

A novel FDTD(2,4) scheme for the simulation of wave propagation inside lossy dispersive materials has been presented. Its stability properties for three specific models have been investigated and appropriate stability conditions have been derived. Additionally, the numerical dispersion characteristics have been examined and for the case of a second-order Lorentz medium, it has been verified that the proposed algorithm is more powerful than the conventional second-order technique, as expected. The efficiency of the FDTD(2,4) algorithm has also been explored in various numerical examples, where it has been compared to the FDTD(2,2) method and an analytical solution. In all the cases considered, it has been proven that the former achieves better accuracy when the same grid is used or the
same level of accuracy for coarser grids. Additionally, the presented method accomplishes minimum errors, while reducing the overall computational time.

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