

Efficient Modelling of Wave Propagation in Lorentz Media via a Controllable (2,4) FDTD Method

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This work presents a finite-difference time-domain (FDTD) scheme that mitigates numerical errors in two-dimensional electromagnetic-wave propagation within Lorentz media. Rather than relying on traditional fourth-order spatial approximations, a new design approach is introduced for the spatial operators that minimizes dispersion flaws along the two principal axes at a specified frequency, affecting simultaneously all possible propagation angles. Performance enhancement over extended frequency bands is also possible in a controllable fashion that involves the least-squares solution of an overdetermined system, derived from single-frequency equations. The results verify that the proposed algorithm outperforms the conventional method without incurring additional computational costs, offering efficient computations for FDTD simulations in dispersive media.

Index Terms—Dispersive media, finite-difference time-domain method, Lorentz model, numerical dispersion.

I. INTRODUCTION

THE DEVELOPMENT of robust finite-difference time-domain (FDTD) techniques [1] for simulating problems with dispersive materials has received significant attention in recent years [2,3]. As with all FDTD methods, numerical dispersion constitutes a primary source of error, which can be mitigated by high-order or optimized discretizations. Notably, recent studies [4,5] demonstrate the successful implementation of dispersion-relation-preserving concepts to such problems that originate from FDTD formulations designed for non-dispersive media.

Focusing on wave-propagation problems in two-dimensional (2D) spaces with material dispersion, we devise an enhanced FDTD algorithm with reduced errors that is suitable for Lorentz media. The improved accuracy arises from the modification of the four-point spatial approximations, which assures error minimization along the two main axes. This specific-frequency design is further extended to broader frequency bands, by formulating and solving an overdetermined system of linear equations via the least-squares method. As the proposed algorithm maintains a typical (2,4) discretization framework, the accomplished improvement comes at virtually no extra computational cost and, thus, provides highly efficient and precise discrete models for dispersive material problems.

II. METHODOLOGY

A. Problem description

We consider the development of an FDTD discretization scheme for dispersive media, whose relative permittivity is described by the Lorentz formula:

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{(j\omega)^2 + 2\delta(j\omega) + \omega_0^2}, \quad (1)$$

where $\varepsilon_s, \varepsilon_\infty$ are the relative permittivity values at zero and infinite frequency, respectively, δ is the damping coefficient, ω_0 is the resonance frequency, and $j = \sqrt{-1}$. This frequency-dependent formula is integrated into the time-domain update equations via an auxiliary-differential-equation approach,

similar to [4,5]. To optimize the scheme's performance without altering the computational complexity, a parametric four-point formula is employed to approximate spatial derivatives:

$$\frac{\partial f}{\partial x} \Big|_{i,j} \approx \frac{1}{\Delta x} \sum_{\ell=1}^2 C_{x\ell} \left(f \Big|_{i+\frac{2\ell-1}{2},j} - f \Big|_{i-\frac{2\ell-1}{2},j} \right), \quad (2)$$

with a similar expression applied for $\partial f / \partial y$ (Δx is the spatial step, $C_{x\ell}$ are constant coefficients). Standard second-order expressions are used for time derivatives and, thus, the scheme has a typical (2,4) structure. However, the formal spatial accuracy is not fourth-order, as the $C_{u\ell}$ coefficients ($u = x, y$) are specified using the methodology presented below.

B. Derivation of spatial formulae

Our approach is founded on the proper utilization of the scheme's numerical dispersion relation, which has the form

$$S_x^2(\omega, \tilde{k}, \varphi) + S_y^2(\omega, \tilde{k}, \varphi) = \frac{\tilde{\varepsilon}_r(\omega)}{c_0^2} T^2(\omega), \quad (3)$$

where

$$S_u(\omega, k, \varphi) = -\frac{2j}{\Delta u} \left[C_{u1} \sin\left(\frac{k_u \Delta u}{2}\right) + C_{u2} \sin\left(\frac{3k_u \Delta u}{2}\right) \right] \quad (4)$$

for $u = x, y$, $k_x = k \cos \varphi$, $k_y = k \sin \varphi$, φ denotes the direction of wave propagation, $\tilde{k}$ is the numerical wavenumber, c_0 is the light speed in the vacuum, and

$$\tilde{\varepsilon}_r(\omega) = \varepsilon_\infty + \frac{(\varepsilon_s - \varepsilon_\infty)\omega_0^2}{T^2(\omega) + 2\delta M(\omega)T(\omega) + \omega_0^2}, \quad (5)$$

$$T(\omega) = \frac{2j}{\Delta t} \sin\left(\frac{\omega \Delta t}{2}\right), \quad M(\omega) = \cos\left(\frac{\omega \Delta t}{2}\right). \quad (6)$$

By enforcing $\tilde{k} = k = (\omega / c_0) \sqrt{\varepsilon_r(\omega)}$ at $\varphi = 0$ and $\pi/2$ for a specific frequency ω_d , we obtain

$$S_x(\omega_d, k_d, 0) = \frac{\sqrt{\tilde{\varepsilon}_r(\omega_d)}}{c_0} T(\omega_d), \quad S_y(\omega_d, k_d, \frac{\pi}{2}) = \frac{\sqrt{\tilde{\varepsilon}_r(\omega_d)}}{c_0} T(\omega_d).$$

Each of these equations has two real unknowns and complex coefficients. Hence, by taking the real and imaginary parts of

each side, two systems are deduced that determine the optimum spatial formula at the selected ω_d :

$$\begin{bmatrix} \text{Re}\left\{\sin\left(\frac{k_d \Delta u}{2}\right)\right\} & \text{Re}\left\{\sin\left(\frac{3k_d \Delta u}{2}\right)\right\} \\ \text{Im}\left\{\sin\left(\frac{k_d \Delta u}{2}\right)\right\} & \text{Im}\left\{\sin\left(\frac{3k_d \Delta u}{2}\right)\right\} \end{bmatrix} \begin{bmatrix} C_{u1} \\ C_{u2} \end{bmatrix} = \frac{\Delta u}{c_0 \Delta t} \sin\left(\frac{\omega_d \Delta t}{2}\right) \begin{bmatrix} \text{Re}\left\{\sqrt{\tilde{\epsilon}_r(\omega_d)}\right\} \\ \text{Im}\left\{\sqrt{\tilde{\epsilon}_r(\omega_d)}\right\} \end{bmatrix}$$

for $u = x, y$. In this way, the dispersion error is minimized along the x - and y -axis, affecting at the same time all the remaining directions of propagation, as we will demonstrate later.

Evidently, the described procedure affects the dispersion error at the chosen frequency ω_d . If further control of the error over an extended range of frequencies is desired, the aforementioned equations need to be satisfied at more than one frequency points. We essentially modify the technique from [4], which considers media with $\delta \rightarrow 0$, and assume that the desired band is covered by N frequencies $\omega_1, \dots, \omega_N$. An overdetermined system $[\mathbf{Z}][\mathbf{c}] = [\mathbf{b}]$ is then defined, where

$$[\mathbf{Z}] = \begin{bmatrix} \text{Re}\{[\mathbf{Z}_c]\} \\ \text{Im}\{[\mathbf{Z}_c]\} \end{bmatrix}, [\mathbf{b}] = \begin{bmatrix} \text{Re}\{[\mathbf{b}_c]\} \\ \text{Im}\{[\mathbf{b}_c]\} \end{bmatrix} \quad (7)$$

$$[\mathbf{Z}_c] = \begin{bmatrix} \sin\left(\frac{k_1 \Delta u}{2}\right) & \sin\left(\frac{3k_1 \Delta u}{2}\right) \\ \vdots & \vdots \\ \sin\left(\frac{k_N \Delta u}{2}\right) & \sin\left(\frac{3k_N \Delta u}{2}\right) \end{bmatrix}, [\mathbf{b}_c] = \frac{\Delta u}{\Delta t} \begin{bmatrix} \sin\left(\frac{\omega_1 \Delta t}{2}\right) \sqrt{\tilde{\epsilon}_r(\omega_1)} \\ \vdots \\ \sin\left(\frac{\omega_N \Delta t}{2}\right) \sqrt{\tilde{\epsilon}_r(\omega_N)} \end{bmatrix} \quad (8)$$

and $[\mathbf{c}] = [C_{u1} \ C_{u2}]^T$, $u = x, y$. The well-known formula $[\mathbf{c}]_{\text{LS}} = ([\mathbf{Z}]^T [\mathbf{Z}])^{-1} [\mathbf{Z}]^T [\mathbf{b}]$ computes the least-squares solution, which specifies spatial formulae with the desired wideband features.

III. RESULTS

The performance of the proposed method is assessed in this section by computing the overall error

$$E_{2D}(\omega) = \frac{1}{2\pi} \int_0^{2\pi} |1 - \tilde{k}(\omega, \varphi) / k(\omega)| d\varphi, \quad (9)$$

when the material parameters are $\epsilon_s = 5.25$, $\epsilon_\infty = 2.25$ and $\delta = 0.1\omega_0$. Comparisons are performed against the standard (2,4) FDTD scheme ($C_{u1} = 9/8$, $C_{u2} = -1/24$), when the mesh density corresponds to 20 cells per wavelength at $\omega = 0.8\omega_0$. First, the coefficients are computed at a specific frequency ($0.7\omega_0$, $1.25\omega_0$, or $2.5\omega_0$) and the corresponding error curves are plotted in the frequency range $0.1\omega_0 - 3\omega_0$ in Fig. 1. The results affirm that the optimization along the two axes suffices to ensure a reduction of the error, as overall accuracy is clearly improved in the proximity of the design points.

Next, the wideband performance of the new method is tested within different frequency bands. Specifically, Fig. 2 compares the overall error E_{2D} of the standard and the proposed FDTD scheme in six different bands, namely $0.2\omega_0 - 0.8\omega_0$, $\omega_0 - 1.5\omega_0$, $1.8\omega_0 - 3\omega_0$, $0.5\omega_0 - 1.5\omega_0$, $1.2\omega_0 - 2.5\omega_0$, and $0.5\omega_0 - 2.5\omega_0$. It becomes apparent that the modified schemes are more reliable than the standard (2,4) version throughout the entire or the biggest part of the bands of interest. Degradation may be occasionally observed at low frequencies. However, this should not be considered a major weakness, as the impact of dispersion errors is not pronounced in this part of the spectrum.

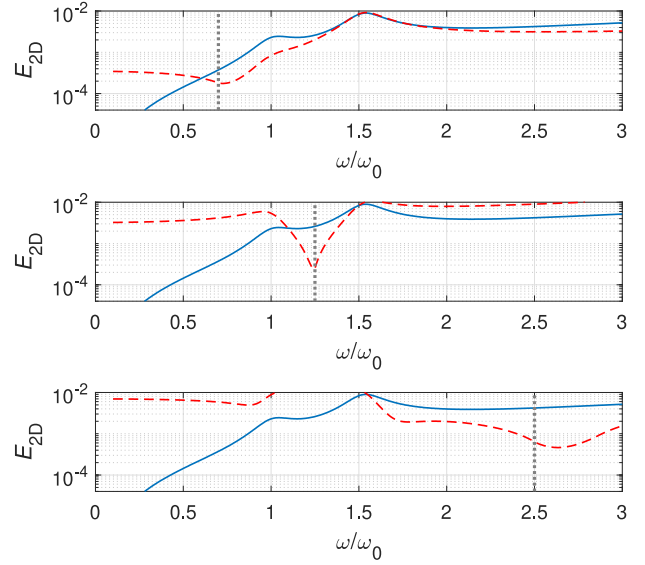


Fig. 1. Error E_{2D} versus normalized frequency, for different design frequencies, denoted by the gray dotted line (blue solid line: standard method, red dashed line: proposed method).

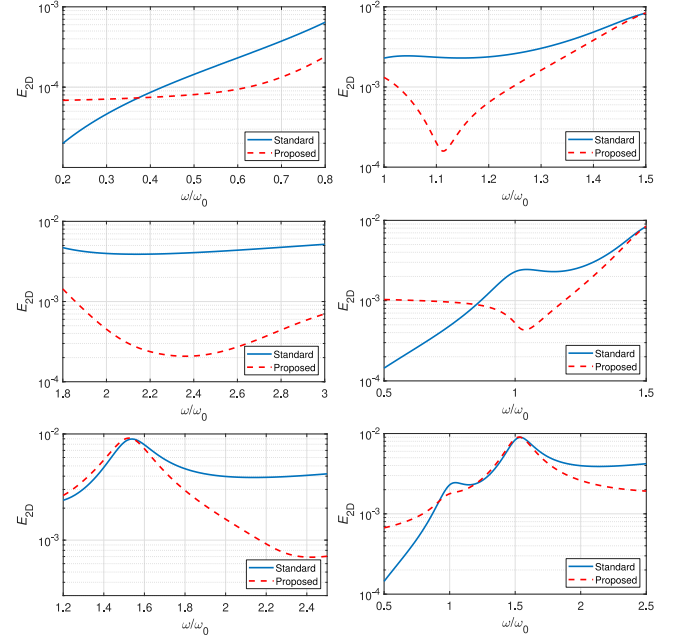


Fig. 2. Error E_{2D} versus normalized frequency, for different design bands. The new method is optimized within the band described by the horizontal axis.

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