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Dispersion Analysis in Time-Domain Simulation of Complex Dispersive Media

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Abstract — Inherent to time-domain method that use space-time discretization, the model dispersion produces field propagation velocity error. In methods such as finite-differences or TLM in time domain, it is customary to choose a maximum mesh size of one tenth of the minimum operating wavelength. If this criterion is easily applicable for normal ordinary media, it is more ambiguous to give interpretation of the wavelength when dealing with complex media such as anisotropic and/or dispersive (frequency dependent) media. After describing the procedure to evaluate dispersion in such media, the paper shows examples for which the simple rule underestimates the maximum mesh size and, consequently, increases the computing expenditure.

Index Terms — Time-domain, Transmission-Line Matrix, dispersion, complex media, velocity error.

I. INTRODUCTION

Volumic computational methods such as FDTD [1] or Transmission-Line Matrix method (TLM) [2] are widely used for full-wave simulation of structures with arbitrary geometry. While FDTD is a direct discretization of curl Maxwell's equation using finite-difference operators, TLM is seen as a discretized version of Huygens' principle of wave propagation. Fields are computed by linear combination of local ordinary waves [2]. Local medium properties are accounted for by correcting the field values at every time step in a way that can be fundamentally described by a filtering process [3]. Generally, the Symmetrical Condensed Node (SCN) proposed by Johns [2] is used, owing to its very good dispersion characteristics (no dispersion in the Cartesian axis directions) and the fact that it always operates at the maximum time-step, computes all field components at the cell center and at the same time-step. Another advantage of the SCN is that continuity of tangential field components is automatically enforced at interfaces between media. As a result, SCN-TLM remains very accurate for high contrast of constitutive parameters [4]. The price to pay is a larger computer expenditure per iteration than when using FDTD, for instance. However, some recent work have shown that, even if the SCN-TLM requires more operations and storage, it substantially outperforms FDTD in terms of computer cost for high contrasted media or zones with irregular mesh with large mesh size difference [5]. This is due to the local properties of the SCN-TLM.

As far as TLM dispersion is concerned, some analyses were reported for non-dispersive media [6]. However, very little work has been reported for complex general media.

In this paper, we present the analytical derivation of a 3D dispersion equation in continuous media. Then, in section III we revisit the formulation done in [3] and reformulate it in matrix form and with Hilbert space representation [6] for general linear media (dispersive, nonhomogeneous, anisotropic, and magneto-electric). In sections IV we derive the TLM scheme dispersion relations. In section V, two examples of dispersion analysis are presented to verify the proposed approach. Finally, it is shown that the procedure for choosing the maximum mesh size is necessary when we dealing with complex media and that commonly used empirical formulas are generally not valid.

II. BASIC THEORY

Time-domain Maxwell's equations for general linear media is given by [3]:

$$\begin{pmatrix} \nabla \times \vec{H} \\ -\nabla \times \vec{E} \end{pmatrix} = \frac{\partial}{\partial t} \begin{pmatrix} \epsilon_0 \vec{E} \\ \mu_0 \vec{H} \end{pmatrix} + \vec{\sigma} * \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix} + \frac{\partial}{\partial t} [\vec{M} * \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix}] + \begin{pmatrix} \vec{J}_{im} \\ \vec{J}_{ie} \end{pmatrix} \quad (1)$$

where * denotes time convolution, $\vec{\sigma}$ represents the conductivity tensor:

$$\vec{\sigma} = \begin{pmatrix} \vec{\sigma}_e & \vec{0} \\ \vec{0} & \vec{\sigma}_m \end{pmatrix} \quad (2)$$

and the matrix \vec{M}

$$\vec{M} = \begin{pmatrix} \vec{\chi}_e & \vec{\xi} \\ \vec{\zeta} & \vec{\chi}_m \end{pmatrix} \quad (3)$$

that includes the electric susceptibility $\vec{\chi}_e$, magnetic susceptibility $\vec{\chi}_m$, and electric-magnetic coupling factors $\vec{\xi}, \vec{\zeta}$, an effect that appears in modeling time varying media such as moving plasma [3]. Finally, $\vec{J}_{ie}, \vec{J}_{im}$ are the electric and magnetic impressed current sources, respectively. Note that $\vec{\sigma}$ takes into account the possible presence of magnetic fictitious free charges [3].

To study the theoretical dispersion characteristics, we should find a relation between the frequency ω , and the wave vector \vec{k} of a wave propagating in the medium. This will allow us to evaluate the wave velocity for a given frequency, as a function of its direction of propagation. It is a way to characterize the numerical model anisotropy. In the same time, the dispersion as a function of frequency for a given direction of propagation can be established. The first step is to write Maxwell's equations (1) for such a wave in spectral domain,

assuming that the medium under study is source free. Hence, we obtain:

$$(\omega \bar{I}_6 + \omega \bar{M}(\omega) - j\bar{\sigma}(\omega) + \bar{\Lambda}) \begin{pmatrix} \vec{E} \\ \vec{H} \end{pmatrix} = 0 \quad (4)$$

where $\bar{\Lambda}$ represents the wave curl operator in spectral domain

$$\bar{\Lambda} = \begin{pmatrix} 0 & 0 & 0 & 0 & +k_z & -k_y \\ 0 & 0 & 0 & -k_z & 0 & +k_x \\ 0 & 0 & 0 & +k_y & -k_x & 0 \\ 0 & -k_z & +k_y & 0 & 0 & 0 \\ +k_z & 0 & -k_x & 0 & 0 & 0 \\ -k_y & +k_x & 0 & 0 & 0 & 0 \end{pmatrix} \quad (5)$$

The necessary condition for (4) to have a nontrivial solution is:

$$\det(\omega \bar{I}_6 + \omega \bar{M}(\omega) - j\bar{\sigma}(\omega) + \bar{\Lambda}) = 0 \quad (6)$$

from which the dispersion relation \vec{k} vs ω can be found.

III. MATHEMATICAL MODEL OF TLM FOR COMPLEX MEDIA

As a first step, we reformulate the TLM algorithm for complex media presented in [3] into a matrix form, in which the field-evolution process is split into 4 steps.

The full derivation of the expressions below is obtained directly from discretized Maxwell's curl equations (1), rearranging the update equations and applying the SCN-based TLM algorithm presented in [7]. Full derivations and other details could be found in [3][7].

A. Propagation Process

Initially, fields at the center of each cell are calculated as a linear combination of the incident voltages from the adjacent cells:

$$\bar{F}_{o,n} = \bar{Q} \bar{V}_{in,n} \quad (7)$$

where $\bar{F}_{o,n}$, $\bar{V}_{in,n}$ are the fields and incident voltages vectors at n -th time step, respectively.

B. Correction Process

After calculating fields at the center of each node as described by (7), local material presence is accounted for by applying a convolution process with a 6×6 correction matrix $\bar{\Gamma}(z)$, whose components are usually filter functions.

Note that the interactions between fields and complex media, translates to convolution products in the time-domain.

$$\bar{F}'_{c,n} = \bar{\Gamma}(z) * \bar{F}_{o,n} \quad (8)$$

where $\bar{F}'_{c,n}$ is the corrected fields vector at the n -th time step.

C. Scattering Process

Once the correction process is completed, the reflected voltages from the 18 ports of each cell in the TLM computational domain are calculated. They will be used later to evaluate the incident voltages to the neighboring cells at the

next time step. The reflected voltages can be expressed as a linear combination of the corrected fields at the center of the cell and the incident voltages at the same time step. This writes in matrix form:

$$\bar{V}_{r,n} = \bar{\Lambda} \bar{F}'_{c,n} - \bar{\Phi} \bar{V}_{in,n} \quad (9)$$

where, the operators $\bar{\Lambda}$, $\bar{\Phi}$ are rectangular matrices [3].

D. Connection Process

After scattering processes took place at every TLM node, arm reflected voltages from one cell become incident voltages to its neighboring ones. This process, which can be seen as a discrete form of Huygens principles of wave propagation, is called the TLM connection process and it can be written as follows [2] [3]:

$$\bar{V}_{in,n+1} = \bar{\Psi} \bar{V}_n \quad (10)$$

where the Hermetian spatial shift operator $\bar{\Psi}$ is defined as:

$$\bar{\Psi} = \begin{pmatrix} 0 & \bar{\psi}_1^\dagger & 0 \\ \bar{\psi}_1 & 0 & 0 \\ 0 & 0 & \bar{I}_6 \end{pmatrix} \quad (11)$$

where the matrix $\bar{\psi}_1$ is defined by:

$$\bar{\psi}_1 = \begin{pmatrix} 0 & 0 & 0 & 0 & Y & 0 \\ 0 & 0 & 0 & Z & 0 & 0 \\ 0 & Z & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & X \\ 0 & 0 & X & 0 & 0 & 0 \\ Y & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (12)$$

and the matrix elements are defined in Table I below.

TABLE I
SPACE-SHIFT OPERATORS IN SPECTRAL DOMAIN AND HILBERT SPACE

Spectral domain notation	Hilbert stappe notation
$X^\dagger = e^{-j\chi}$	$X^\dagger n; k, l, m\rangle = n; k-1, l, m\rangle$
$X = e^{j\chi}$	$X n; k, l, m\rangle = n; k+1, l, m\rangle$
$Y^\dagger = e^{-j\eta}$	$Y^\dagger n; k, l, m\rangle = n; k, l-1, m\rangle$
$Y = e^{j\eta}$	$Y n; k, l, m\rangle = n; k, l+1, m\rangle$
$Z^\dagger = e^{-j\xi}$	$Z^\dagger n; k, l, m\rangle = n; k, l, m-1\rangle$
$Z = e^{j\xi}$	$Z n; k, l, m\rangle = n; k, l, m+1\rangle$

where χ , η , ξ are the normalized spatial frequencies. They are defined by:

$$\chi = 2\pi\Delta x k_x \quad (13.a)$$

$$\eta = 2\pi\Delta y k_y \quad (13.b)$$

$$\xi = 2\pi\Delta z k_z \quad (13.c)$$

III. DISPERSION ANALYSIS

As shown earlier in section II for continuous media, the relationship between operating frequency and wave vector (6), is the dispersion relation. For a discrete computational scheme, the procedure is similar. First, we express the update equations in spectral domain using Hilbert space representation. Then, by constructing a homogeneous linear system similar to (4), the condition for nontrivial solutions yields eigen values and associated eigen functions. Starting from the simple observation

$$\bar{F}_{o,n} = \bar{T}\bar{F}_{o,n-1} \quad (14)$$

where \bar{T} is the time shift operator. It increments the time index by one step value for all cells in the computational domain:

$$\bar{T} |n+1; k, l, m\rangle = |n; k, l, m\rangle \quad (15)$$

or in matrix form :

$$\bar{T} = e^{j\Omega} \bar{I}_{18} \quad (16a)$$

where the normalized frequency Ω is defined as:

$$\Omega = 2\pi\Delta t f \quad (16b)$$

by combining (8), (9) and (10) we obtain:

$$\bar{V}_{in,n} = \bar{\Psi}(\bar{\Lambda}\bar{\Gamma} * \bar{F}_{o,n-1} - \bar{\Phi}\bar{V}_{in,n-1}) \quad (17a)$$

Using (7), and the time shift operation (14) in (17a), yields the eigenvalue equation:

$$\bar{T}\bar{V}_{in,n-1} = \bar{\Psi}(\bar{\Lambda}\bar{\Gamma}(z)\bar{Q}\bar{V}_{in,n-1} - \bar{\Phi}\bar{V}_{in,n-1}) \quad (17b)$$

This allows one to obtain the dispersion relation for discrete TLM model for complex media is follows:

$$\det(\bar{T} - \bar{\Psi}(\bar{\Lambda}\bar{\Gamma}(z)\bar{Q} - \bar{\Phi})) = 0 \quad (18)$$

In most publications, either for FDTD or TLM [1, 7], authors use the following inequality as a rule to calculate the maximum cell size that maintains some acceptable level of dispersion:

$$\{\Delta x, \Delta y, \Delta z\} \leq \text{Min} \left[\frac{\lambda_o}{10\sqrt{\epsilon_r\mu_r}} \right] \quad (19)$$

where λ_o is the wavelength in free space, ϵ_r, μ_r are the permittivity and the permeability of the medium, respectively. Whenever, the computational domain consists of nonhomogeneous media (which is usually the case), one should use the minimum cell dimension, so that the overall dispersion will remain negligible everywhere, and this is the reason behind the *Min* operator in (19). As a matter of fact, this relation (which agrees with the approach presented earlier) is trustful only for isotropic nondispersive lossless media. However, when complex media are involved and when it is necessary not to exceed a certain limit of dispersion, a mesh convergence test should be applied. This implies that successive simulations from a coarser to a finer mesh should be performed, at least at some locations.

The alternative to a mesh convergence test is to know the level of dispersion a priori, by solving (18). Therefore, one

can use a maximum cell size in all regions which does not require fine spatial resolution.

IV. RESULTS AND DISCUSSIONS

In this section we present an experiment considering a nonmagnetic Lorentz medium, with permittivity defined as [8]:

$$\bar{\epsilon}_r(\omega) = \left(\epsilon_\infty + \frac{(\epsilon_s - \epsilon_\infty)\omega_o^2}{\omega_o^2 - \omega^2 + 2j\zeta_e\omega} \right) \bar{I}_3 \quad (20)$$

where ω_o is the characteristic resonant frequency of the Lorentz material sample, ζ_e the damping coefficient, ϵ_s the static value of permittivity and ϵ_∞ is the value at high frequencies.

In Fig. 1, the dispersion curves for different values of operating frequency ω are presented V_{PN} is the numerical phase velocity and V_{PT} is the theoretical phase velocity .

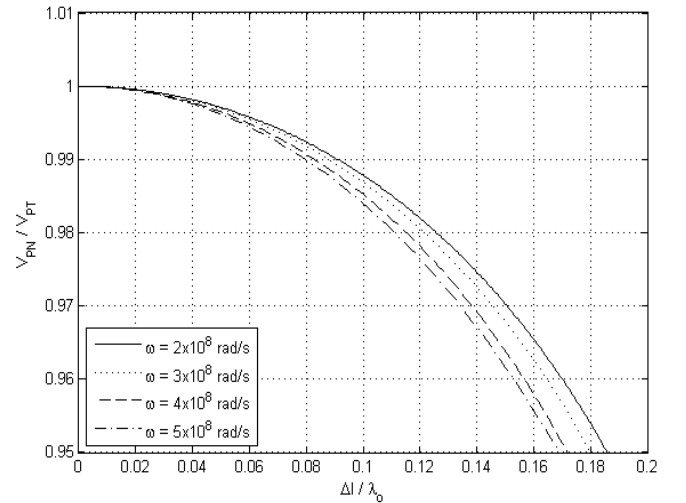


Fig. 1, numerical dispersion curves in Lorentz medium along the cell diagonal direction (1,1,1), with parameters, $\epsilon_s = 2$, $\epsilon_\infty = 1$, $\omega_o = 6 \times 10^8 \text{ rad/s}$ and $\zeta_e = 0.167 \omega_o$

As observed in Fig.1, the dispersion characteristics changes according the operating frequency ω due to the fact that the material properties are also changing. Table II shows the difference between using (19) as a rough estimation for the maximum spatial step, and using the proposed approach with 1.0 % error criteria.

TABLE II

COMPARISON BETWEEN THE RIGOROUS PROPOSED APPROACH AND THE RULE (19) FOR MAXIMUM CELL SIZE IN TERMS OF MEMORY REQUIREMENTS FOR THE LORENTZ MEDIUM (20), CASE OF FIG. 1

Frequency (10^8 rad/s)	$\Delta l / \lambda_o$ Formula (19)	$\Delta l / \lambda_o$ 1.0% Error	Memory saving %	CPU time saving %
2.0	0.0688	0.0914	234.5 %	311.5 %
3.0	0.0661	0.0871	228.8 %	301.5 %
4.0	0.0617	0.0828	241.7 %	324.3 %
5.0	0.0556	0.0791	287.9 %	406.6 %

It is obvious that using this approach, one can control the level of dispersion to the desired value but with some compromise with the computational requirements. For instance, fixing the maximum level of dispersion to 1.0%, leads to more than half the computational effort compared to the rule (19).

In the second experiment, we chose a nonmagnetic, lossless biaxial medium [9] defined by:

$$\bar{\bar{\epsilon}}_r = \begin{pmatrix} \epsilon_x & 0 & 0 \\ 0 & \epsilon_y & 0 \\ 0 & 0 & \epsilon_z \end{pmatrix} \quad (21)$$

The operating frequency $f = 500 \text{ MHz}$, and Δt_{max} [10] was used. As shown in Fig.2, different directions have different dispersion characteristics. For instance, in x-direction no dispersion appears, whereas, a maximum dispersion occurs along the main diagonal direction of the cube (1,1,1).

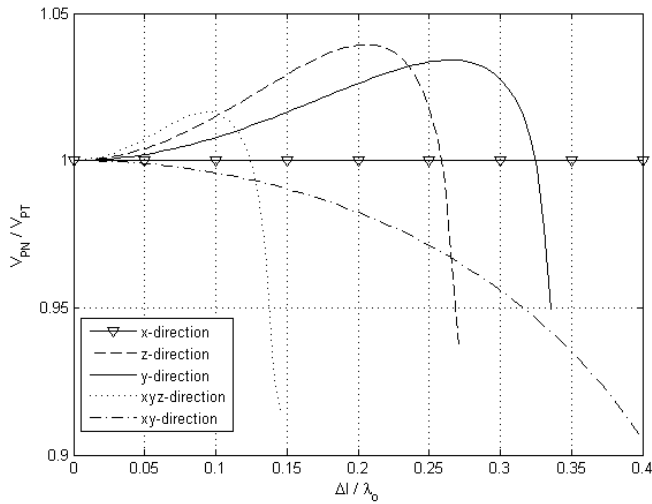


Fig. 2, dispersion curves in a nonmagnetic anisotropic medium at different directions of propagation, where $\bar{\bar{\epsilon}}_r = \text{diag}\{1,2,3\}$

If one chooses an empirical formula such as (19), then the maximum spatial step will be $\lambda_0/10\sqrt{\epsilon_{r,Max}} = 0.057 \lambda_0$, for a negligible dispersion error, which matches results in Fig.2 for around 1.0% error threshold. However, for general anisotropic media with non-zero out of diagonal elements the empirical formula (19) fails to predict the appropriate value (can be either too big or too small) of mesh size whereas our approach remains valid and gives the appropriate mesh size corresponding to the level of dispersion error fixed in priori.

V. CONCLUSION

In this paper, a procedure to evaluate dispersion characteristics was presented for the TLM-SCN algorithm for

general linear media. A similar approach can be applied for FDTD or FIT (Finite Integration Technique) algorithms. It is only necessary to modify the corresponding update equations.

In the result section, a numerical experiment was presented to show the validity of the SCN-TLM approach for complex medium. Furthermore, for complex media no formulas are available for evaluating both maximum space and time steps. It is shown that the procedure allows one to select optimum values which leads to efficient simulation: minimizing both the dispersion error and the computer expenditure. Finally, the procedure described here is valid for any linear, anisotropic, dispersive medium for field computation by the time-domain TLM model.

This procedure presented in this paper can be similarly applied to other time-domain computational methods.

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