Finite Difference Time Domain Modeling of General Dispersive Bi-Isotropic Media

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Abstract: In this paper we present a novel Finite Difference Time Domain (FDTD) model of *transient* wave propagation in *general dispersive bi-isotropic media*. Much attention has been focused recently on the behavior of these materials and their potential applications in microwave and millimetre–wave technology. While these materials have been extensively studied in the frequency domain, their time domain behavior has only been modeled so far for *special sub-classes* or *time harmonic operation*. To validate our method we have computed the behavior of electromagnetic waves traveling through a bi-isotropic medium and compared it with theoretical results. Agreement is typically better than one percent.

1 Introduction

Bi-isotropic materials contain two additional parameters in their constitutive equations, namely the *Tellegen* and *chirality* parameters, that relate the electric field E with the magnetic flux density B, and the magnetic field H with the electric displacement D. Electromagnetic waves in bi-isotropic media show the following interesting behavior [1]:

a) **Optical Rotatory Dispersion** causing a **rotation of polarization**;
b) **Circular Dichroism***,* which modifies the nature of field polarization (lossy case);
c) **Non-orthogonality of electric and magnetic field vectors** and **dependency of the phase velocity** on the *Tellegen* parameter.

Two subclasses of general bi-isotropic media are *Tellegen* and *Chiral* media, in which only one of these two parameters is taken into account in the constitutive equations. Several time domain models of bi-isotropic media have been published [2] [3] [4] for special cases, such as chiral media, non-dispersive bi-isotropic media, or time-harmonic operation. However, no *transient* time domain formulation has been developed to date that models *general bi-isotropic dispersive media*. In this work a full time-domain model of general bi-isotropic dispersive media is presented. It is based on the FDTD technique, where the basic Yee cell has been modified to include the special relationships between the field vectors in bi-isotropic media. To validate our method we have computed the characteristic behavior of electromagnetic waves traveling through a bi-isotropic medium and obtained very good agreement with theory.

2 Time Domain Constitutive Equations in Bi-Isotropic Media

The constitutive equations for bi-isotropic media in frequency domain are given by [1]:

$$\begin{aligned}\vec{D}(\omega) &= \varepsilon\vec{E}(\omega) + \sqrt{\varepsilon_0\mu_0}\left(\chi - j\kappa(\omega)\right)\vec{H}(\omega)\\ \vec{B}(\omega) &= \mu\vec{H}(\omega) + \sqrt{\varepsilon_0\mu_0}\left(\chi + j\kappa(\omega)\right)\vec{E}(\omega)\end{aligned} \tag{1}$$

where χ is the *Tellegen* parameter and $\kappa(\omega)$ is the frequency-dependent *chirality* parameter.

The frequency behavior of the chirality parameter is assumed to follow the Condon [1], [5] model with one dominant resonance that lies far away from other molecular transitions. Hence, the frequency dependence of the chirality parameter can be written as:

$$\kappa(\omega) = \frac{\tau\omega_o^2\omega}{\omega_o^2 - \omega^2 + j2\omega_o\xi\omega} \tag{2}$$

where ω_0, is a characteristic resonant frequency, τ a time constant and ξ a damping factor.

In order to obtain a time domain expression for the chirality parameter, the imaginary unit that appears in the constitutive equations (1) is introduced in the chirality parameter expression (2), and the time-dependent chirality parameter is obtained by inverse Laplace transform:

$$L^{-1}\left(\kappa'(\omega)\right) = \kappa'(t) = \left(\frac{-\tau\omega_0^2\xi}{2\sqrt{\xi^2-1}} + \frac{\tau\omega_0^2}{2}\right)e^{\left[-\xi\omega_0+\omega_0\sqrt{\xi^2-1}\right]t} + \left(\frac{\tau\omega_0^2\xi}{2\sqrt{\xi^2-1}} + \frac{\tau\omega_0^2}{2}\right)e^{\left[-\xi\omega_0-\omega_0\sqrt{\xi^2-1}\right]t} \tag{3}$$

where the new chirality parameter $\kappa'(\omega)$ is defined as $\kappa'(\omega)=j\,\kappa(\omega)$.

For the lossless case ($\xi=0$) the chirality parameter simplifies to:

$$\kappa'(t) = \tau\omega_0^2\cos(\omega_0 t) \tag{4}$$

In time domain the relationship given in eq. (1) becomes a convolution:

$$\begin{aligned} \vec{D}(t) &= \varepsilon\vec{E}(t) + \frac{\chi}{c_0}\vec{H}(t) - \frac{1}{c_0}\int_0^t \kappa'(\tau)\vec{H}(t-\tau)d\tau \\ \vec{B}(t) &= \mu\vec{H}(t) + \frac{\chi}{c_0}\vec{E}(t) + \frac{1}{c_0}\int_0^t \kappa'(\tau)\vec{E}(t-\tau)d\tau \end{aligned} \tag{5}$$

If we discretize these equations and make the approximation that all the field quantities are constant over each discrete time interval, and if we assume that all fields are zero for $t<0$, then the integration becomes in part a summation [6]:

$$\begin{aligned} \vec{D}(n) &= \varepsilon\vec{E}(n) + \frac{\chi}{c_0}\vec{H}(n) - \frac{1}{c_0}\sum_{m=0}^{n}\vec{H}(n-m)\int_{m\Delta t}^{(m+1)\Delta t}\kappa'(\tau)d\tau \\ \vec{B}(n) &= \mu\vec{H}(n) + \frac{\chi}{c_0}\vec{H}(n) + \frac{1}{c_0}\sum_{m=0}^{n}\vec{E}(n-m)\int_{m\Delta t}^{(m+1)\Delta t}\kappa'(\tau)d\tau \end{aligned} \tag{6}$$

In the lossless case the time dependence of the chirality parameter $\kappa'(t)$ given in (4) is not in a form such that the corresponding discrete convolution can be updated recursively. However, if we define a complex time domain chirality [7]:

$$\hat{\kappa}'(t) = \tau\omega_0^2 e^{-j\omega_0 t} \tag{7}$$

so that

$$\kappa'(t) = Re(\hat{\kappa}(t)) \tag{8}$$

where the caret denotes complex quantities and Re( ) is the real operator. Using the notation:

$$\kappa'(m) = \int_{m\Delta t}^{(m+1)\Delta t} \kappa'(\tau)d\tau \tag{9}$$

$$\hat{\kappa}'(m) = \int_{m\Delta t}^{(m+1)\Delta t} \hat{\kappa}'(\tau)d\tau \tag{10}$$

and since $\hat{\kappa}'(m+1)$ can be written as a function of its previous value as $\hat{\kappa}'(m+1) = \hat{\kappa}'(m)e^{-j\omega_0\Delta t}$, the convolution summation can be computed recursively. We denote ${}^{E}\vec{\psi}(n)$ the convolution summation of the electric field with the chiral response of the material to an impulse, at the instant $n\Delta t$:

$${}^{E}\vec{\psi}(n) = \sum_{m=0}^{n} \vec{E}(n-m)\kappa'(m) \tag{11}$$

Therefore, we can also define a complex summation convolution as follows:

$${}^{E}\hat{\vec{\psi}}(n) = \sum_{m=0}^{n} \vec{E}(n-m)\hat{\kappa}'(m) \tag{12}$$

$${}^{E}\vec{\psi}(n) = Re({}^{E}\hat{\vec{\psi}}(n)) \tag{13}$$

The convolution summation ${}^{E}\hat{\vec{\psi}}(n)$ can be computed by updating ${}^{E}\hat{\vec{\psi}}(n-1)$ [7]:

$${}^{E}\hat{\vec{\psi}}(n) = \vec{E}(n)\hat{\kappa}'(0) + \sum_{m=0}^{n-1} \vec{E}(n-m-1)\hat{\kappa}'(m+1) = \vec{E}(n)\hat{\kappa}'(0) + \sum_{m=0}^{n-1} \vec{E}(n-m-1)\hat{\kappa}'(m)e^{-j\omega_0\Delta t} = \vec{E}(n)\hat{\kappa}'(0) + {}^{E}\hat{\vec{\psi}}(n-1)e^{-j\omega_0\Delta t}$$

the final updating equation obtained is:

$${}^{E}\vec{\psi}(n) = \mathrm{Re}\left[{}^{E}\hat{\vec{\psi}}(n)\right] = \mathrm{Re}\left[\vec{E}(n)\hat{\kappa}'(0) + {}^{E}\hat{\vec{\psi}}(n-1)e^{-j\omega_0\Delta t}\right] \tag{14}$$

$${}^{E}\vec{\psi}(n) = \tau\omega_0 \sin(\omega_0\Delta t)\vec{E}(n) + \mathrm{Re}\left[{}^{E}\hat{\vec{\psi}}(n-1)e^{-j\omega_0 t}\right] \tag{15}$$

In the same way, the convolution summation for the magnetic field is also updated recursively from previous values. In the computer program, this will require four complex numbers per cell, two for the *x* and *y* components of the convolution with the electric field, and two for the *x* and *y* components of the convolution with the magnetic field.

Finally, we substitute these expressions in the discretized time domain constitutive equations (6):

$$\begin{aligned}\vec{D}(n) &= \varepsilon\vec{E}(n) + \frac{\chi}{c_0}\vec{H}(n) - \frac{1}{c_0}\left[\tau\omega_0\sin(\omega_0\Delta t)\vec{H}(n) + \mathrm{Re}\left[{}^{H}\hat{\vec{\psi}}(n-1)e^{-j\omega_0\Delta t}\right]\right] \\ \vec{B}(n) &= \mu\vec{H}(n) + \frac{\chi}{c_0}\vec{E}(n) + \frac{1}{c_0}\left[\tau\omega_0\sin(\omega_0\Delta t)\vec{E}(n) + \mathrm{Re}\left[{}^{E}\hat{\vec{\psi}}(n-1)e^{-j\omega_0\Delta t}\right]\right]\end{aligned} \tag{16}$$

3 New FDTD Formulation.

In order to model bi-isotropic media, we have modified the traditional FDTD method. Although we present in this paper only the implementation of a one-dimensional mesh and algorithm, this formulation can be extended to the two- and three-dimensional cases as well. We assume one-dimensional uniform wave propagation in the *z*-direction. In order to capture the rotation of the fields (caused by the chirality parameter) and their non-orthogonality (caused by the *Tellegen* parameter) in the transversal plane, we model the *x*- and *y*-components of both the electric and magnetic fields.

The peculiar constitutive equations of bi-isotropic media that relate the electric and magnetic fields in the same point and at the same time instant, require a modification of the Yee cell and the traditional FDTD algorithm. Our new cell includes four quantities in each node, namely *E, D, H* and *B*, related by the constitutive equations, and we distinguish two different kinds of nodes, the *x-nodes* where we define the *x-components* of the fields (E_x, D_x, H_x, B_x), and the *y-nodes* with the *y-components* (E_y, D_y, H_y, B_y). The *x-nodes* and the *y-nodes* are staggered in space and time, as shown in Figure 1.

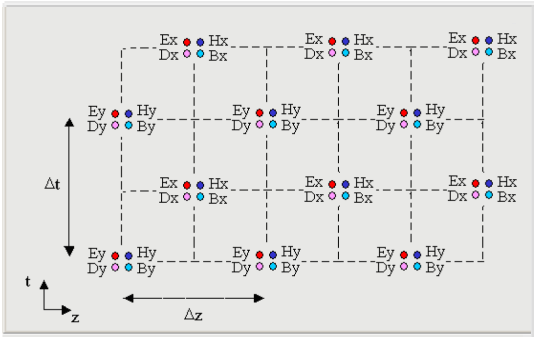

Figure 1. Modified FDTD mesh for bi-isotropic media.

In the following, the updating algorithm for this mesh will be developed. First, we update the *x-components* of the electric displacement *D* and the magnetic flux density *B* everywhere in the mesh by means of the standard FDTD update equations, then, within the *same time step*, the *x-components* of the electric field *E* and the magnetic field *H* are calculated using the *x-component* of the vectorial constitutive equations in time domain (16) derived in the previous section:

$$
\begin{aligned}
D_i^x(n) &= \varepsilon E_i^x(n) + \frac{\chi}{c_0} H_i^x(n) - \frac{1}{c_0}\left[\tau\omega_0 \sin(\omega_0\Delta t) H_i^x(n) + \mathrm{Re}\left[{}^{H}\hat{\psi}_i^x(n-1) e^{-j\omega_0\Delta t}\right]\right] \\
B_i^x(n) &= \mu H_i^x(n) + \frac{\chi}{c_0} E_i^x(n) + \frac{1}{c_0}\left[\tau\omega_0 \sin(\omega_0\Delta t) E_i^x(n) + \mathrm{Re}\left[{}^{E}\hat{\psi}_i^x(n-1) e^{-j\omega_0\Delta t}\right]\right]
\end{aligned}
\tag{17}
$$

At *one half time step* later, the *y-components* of *D* and *B* are computed using the same standard FDTD update equations and, at the *same time step*, we calculate the *y-components* of the electric and magnetic fields using the *y-component* of the vectorial constitutive equations that relate the quantities in our *y-node*:

$$
\begin{aligned}
D_{i+1/2}^y(n+1/2) &= \varepsilon E_{i+1/2}^y(n+1/2) + \frac{\chi}{c_0} H_{i+1/2}^y(n+1/2) - \frac{1}{c_0}\left[\tau\omega_0 \sin(\omega_0\Delta t) H_{i+1/2}^y(n+1/2) + \mathrm{Re}\left[{}^{H}\hat{\psi}_{i+1/2}^y(n-1/2) e^{-j\omega_0\Delta t}\right]\right] \\
B_{i+1/2}^y(n+1/2) &= \mu H_{i+1/2}^y(n+1/2) + \frac{\chi}{c_0} E_{i+1/2}^y(n+1/2) + \frac{1}{c_0}\left[\tau\omega_0 \sin(\omega_0\Delta t) E_{i+1/2}^y(n+1/2) + \mathrm{Re}\left[{}^{E}\hat{\psi}_{i+1/2}^y(n-1/2) e^{-j\omega_0\Delta t}\right]\right]
\end{aligned}
\tag{18}
$$

4 Results

To validate our formulation, we have computed the characteristic behavior of electromagnetic waves traveling through a bi-isotropic medium, and compared it with known theoretical results[1]. As mentioned in the introduction, electromagnetic waves in bi-isotropic lossless media exhibit the following interesting properties [1]:

Optical Rotatory Dispersion causes a **rotation of polarization** due to different phase velocities of the right- and left-handed circularly polarized waves. The sense and angle of rotation depend on the *real part* of the *chirality parameter*.

Non-orthogonality of electric and magnetic field vectors due to the non-zero Tellegen parameter

These properties were simulated in a 1-D computational domain *10,000 cells* (Δz = *1/3 mm*) long. The excitation was applied at the point *4000* Δz, the mesh boundaries were thus far enough so that no reflection appeared in the simulation.

4.1 Rotation of the Polarization and Non-Orthogonality of the Field Vectors

In the first simulation we have computed the rotation of the polarization of an electromagnetic wave propagating in a bi-isotropic medium characterized by the following parameters: $\mu_r = 1$, $\varepsilon_r = 2$, $\chi = 0$, $\tau = 4\ ps$, $\omega_0 = 2\pi\, 10^9\ rad/s$ and $\xi = 0$ (lossless case). To allow comparison with analytical frequency domain results we have injected a time-harmonic electric field (f = *3 GHz*) linearly polarized at *45 degrees* with respect to the *x*- and *y*-axes. At *3 GHz*, the value of the chirality is $\kappa = -\ 9.42 \cdot 10^{-3} + j0$. Since the chirality parameter is real, the wave keeps its linear polarization as it propagates, but due to its negative value, the polarization rotates clockwise when looking in the direction of propagation (+*z* direction) as shows Figure 2. The theoretical angle of rotation of the polarization in a bi-isotropic medium is given by $\alpha = -Re(\kappa) k_0\, z$, where $Re(\kappa)$ is the real part of the chirality parameter, k_0 the wave number in free space, and *z* the distance traveled in the medium.

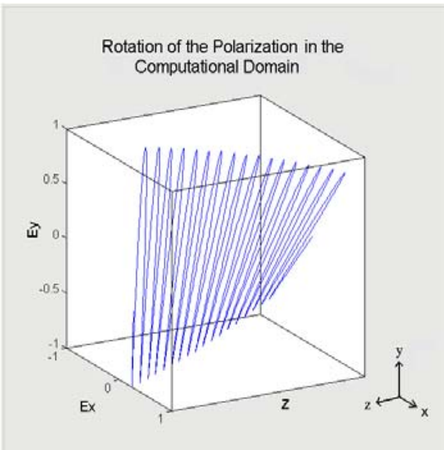

Figure 2. Rotation of the polarization of a wave propagating in a chiral medium. The figure shows the orientation of the electric field in part of the computational domain at time t=4000 ps

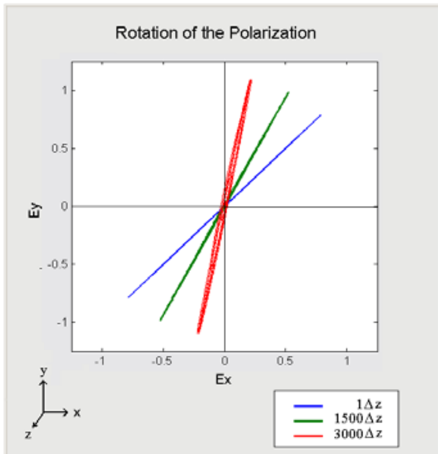

Figure 3. Polarization of the electric field at 1Δz, 1500Δz and 3000Δz from the source. The polarization rotates clockwise as the wave propagates in the medium

In this simulation, we extracted the fields at *1* Δz, *1500* Δz and *3000* Δz from the source, with Δz = *1/3 mm* and Δt = *1ps*. The angle of rotation in these three points is shown in Figure 3. Theoretical and simulated values of the rotation angle are compared in Table 1.

Distance from the source	Theoretical angle of rotation (degrees)	Angle obtained with our FDTD simulation (degrees)	Relative Error in Percent
1500Δz	16.965	17.127	+0.95
3000Δz	33.929	34.158	+0.67

Table 1 Comparison of theoretical and simulated values of the polarization angle rotation in a bi-isotropic medium for two different distances from the source.

We have performed a second simulation in which we have computed the angle between the electric and magnetic field vectors of a wave in a bi-isotropic medium. This angle is determined by χ, and we have computed it for a bi-isotropic medium with parameters: $\mu_r=1$, $\varepsilon_r=2$, $\tau=3\ ps$, $\omega_0= 2\pi\cdot 10^9\ rad/s$ and $\xi=0$ (lossless case) and three different values of the *Tellegen* parameter $\chi=0.1$, $\chi=0.2$, and $\chi=0.3$. Table 2 shows the theoretical and simulated values of the angle between E and H in the *xy*-plane for the different values of χ.

Tellegen parameter	Theoretical angle between E H (degrees)	Angle obtained with our FDTD simulation (degrees)	Relative Error in Percent
χ=0.1	94.055	93.979	-0.08
χ=0.2	98.130	97.985	+0.14
χ=0.3	102.247	102.38	+0.12

Table 2. Comparison of theoretical and simulated values of the angle between the electric and magnetic field vectors in the *xy*-plane in a bi-isotropic medium for three values of the *Tellegen* parameter.

In one last numerical experiment we have chosen a value of $\chi=0.3$ for the Tellegen parameter; the other parameters of the medium and the excitation are the same than in the previous simulation. The result of this experiment is presented in Figure 6, which simultaneously shows the two basic properties of waves propagating in *general lossless bi-isotropic media*, namely rotation of the polarization and non-orthogonality of E and H.This figure shows E and H (multiplied by Z_c) at the points $1\Delta z$, and $3000\ \Delta z$ from the source.

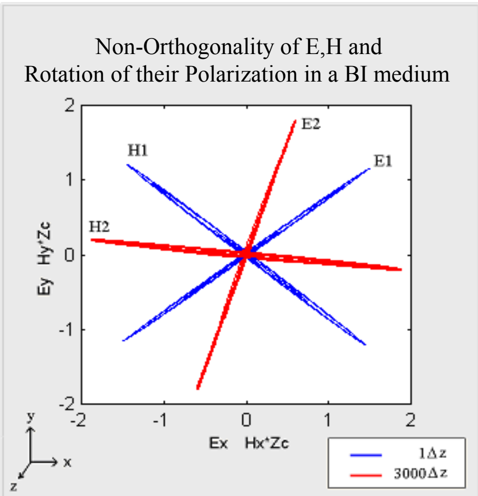

Figure 6. Rotation of the polarization and non-orthogonality of *E* and *H* at the points $1\Delta z$, and $3000\Delta z$ from the source. The polarization is rotated clockwise (looking in the direction of propagation) as the wave propagates in positive *z*-direction. The *Tellegen* parameter fixes the angle between *E* and *H* to *102 degrees*

4.2 Phase Velocity of the Eigenwaves

In bi-isotropic media, fields can be decomposed into two eigenwaves E^+, H^+ and E^-, H^- where "+" designates right-handed circular polarization (CP^+) and "-" left-handed circular polarization (CP^-). Each of these eigenwaves has a different phase velocity what yields to the rotation of the polarization shown in the previous simulations.

In this experiment we have simulated the phase velocities of the CP^+ and CP^- eigenwaves separately. The medium is described by the parameters: $\mu_r=1$, $\varepsilon_r=3$, $\chi=0.2$, $\tau=3\ ps$, $\omega_0=2\pi\ 10^9\ rad/s$ and $\xi=0$ (lossless case), and the source excites a left- and right-handed circularly polarized electric field ($\omega_0 = 2\pi \cdot 3 \cdot 10^9$ *rad/s*), respectively. Table 3 compares the theoretical and simulated values of both phase and velocities.

	Theoretical value (m/s)	Value obtained with our FDTD simulation (m/s)	Relative Error in Percent
Phase velocity CP^+	$2.152 \cdot 10^8 = 0.718 \cdot c$	$2.144 \cdot 10^8 = 0.715 \cdot c$	-0.41
Phase velocity CP^-	$2.131 \cdot 10^8 = 0.711 \cdot c$	$2.142 \cdot 10^8 = 0.714 \cdot c$	+0.54

Table 3. Comparison of theoretical and simulated values of the phase velocity of the right- and left-handed circularly polarized eigenwaves in a bi-isotropic medium.

5 Conclusions

We have presented a novel time domain model of wave propagation in *general dispersive bi-isotropic* media, assuming a Condon model for the chirality parameter, and formulating the constitutive relationships by recursive convolution. To model the peculiar constitutive equations of bi-isotropic media we have modified the traditional FDTD method and Yee cell such that the new formulation presented here involves updating electric and magnetic fields in the same point and at the same time step. While this model has been implemented and validated here for the 1-D case only, it can easily be extended to the two- and three-dimensional cases as well. To our knowledge this is the first time domain formulation that allows full transient modeling of *general dispersive bi-isotropic* media.

The validity and accuracy of the proposed algorithm have been tested in a series of numerical experiments where we have successfully simulated the characteristic behavior of wave propagation in *general dispersive bi-isotropic media.* Simulated rotation angles and phase velocities agree with theoretical values within typically less than one percent.

6 References

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