A novel approach for modeling and simulation of electromagnetic waves in anisotropic dielectrics

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Abstract

The main object of this paper is the initial value problem for the time-dependent Maxwell’s system with tensor dielectric permittivity describing the electromagnetic wave propagation in anisotropic dielectrics. Using the symbolic and algebraic computations in MATLAB a new method of constructing the exact solution of this initial value problem is obtained. The collection of images of electromagnetic waves in different anisotropic dielectrics is created by this method. This collection can be used for the study of properties of anisotropic dielectrics and evaluation of different computational methods.

Keywords: Anisotropic dielectrics; Time-dependent Maxwell’s system; Initial value problem; Simulation; Electromagnetic wave propagation; Symbolic and algebraic computations

1. Introduction

Electromagnetic wave propagation inside of different materials has attracted a great deal of interests in the past decades (Ramo et al., 1994; Monk, 2003; Cohen et al., 2003; Yakhno, 1998). Nowadays the development of new smart materials, in particular anisotropic, stimulates a new interest to modeling and simulating these wave phenomena (Ting, 1996; Ting et al., 1990; Fedorov, 1968; Yakhno and Merazhov, 2000).

Large scale computer modeling can help to understand the properties of these materials and the simulation results can guide the development of more practical ones. For instance, using the theory of an initial...
value problem for the system of elasticity with polynomial data Yakhno and Akmaz (2005a,b) have developed a method for modeling and simulating waves in anisotropic elastic materials. Another method for constructing Green’s matrix-function for the time-dependent Maxwell’s system in anisotropic dielectrics was suggested by Yakhno (2005).

Most of the time the numerical methods, in particular finite element method, have been used to deal with electromagnetic wave propagation. Numerical methods rule supreme thanks to the truly remarkable advances in computing power over the last decades (Monk, 2003; Cohen, 2002; Cohen et al., 2003). Advantages and disadvantages of these methods are well known (see, for example, Zienkiewicz and Taylor, 2000; Monk, 2003; Cohen et al., 2003). Generally speaking, they are of a general purpose, rather labor-consuming, find approximate solutions, but do not always satisfy engineers at the needed scale and accuracy (Pavlovic, 2003).

At the same time classical analytical techniques can provide the exact solution of the equations and also offer a fundamental understanding of the relevant physical phenomena. Unfortunately the exact solutions cannot be found for all complex equations and systems. But when the exact solutions can be found it leads to the significant simplification of modeling and simulation. In general, because of the complexity of mathematical models the analytical formulae are very often boundless and cumbersome that it becomes almost impossible to calculate them ‘by hand’. At this point the modern methods of symbolic and algebraic computations, known as Computer Algebra, allow us to automate mathematical transformations on a very high level of complexity and combine mathematics with advanced computing techniques. The usefulness of symbolic computations in different area of engineering has steadily been recognized (Pavlovic, 2003; Beltzer, 1990; Pavlovic and Sapountzakis, 1986). On the whole, the resulting computer systems using explicit symbolic formulae for modeling and simulation are powerful tools for scientists and engineers.

Without questioning the dominance of numerical methods in present day practice our paper points the advantages of the analytical approach in engineering and scientific computations. In our paper we present a novel approach for modeling and simulation of electromagnetic waves propagation in anisotropic dielectrics. This approach is based on finding an exact solution of the initial value problem (IVP) for Maxwell’s system with the tensor dielectric permittivity and consists in two parts: first, constructing the Fourier image of IVP solution and, second, finding the inverse Fourier transform of this image. The Fourier image here is related to the Fourier transform with respect to 3-D space variable. The different properties of matrix transformations are widely used in the first step for the Fourier image of IVP solution. The explicit formulae obtained in this step are very cumbersome. At this point symbolic computations help us to get the exact Fourier image of the solution. In the next step we have to calculate 3-D inverse Fourier transform of the obtained image. The complexity of the formula for the Fourier image of IVP solution containing four independent variables makes the symbolic calculation of the inverse Fourier transform impracticable. That was the reason why numerical calculation of the inverse Fourier transform was realized on this step. The obtained exact solutions were used for a computer simulation of electromagnetic waves propagation in different dielectrics. As a result of this simulation we created a collection of images of electric wave propagation in different anisotropic dielectrics. This collection is organized as a library which can be used for classification of these materials and evaluation of different computational methods.

The paper is organized as follows. In Section 2 we specify the time-dependent Maxwell’s system which we will use as a mathematical model of electromagnetic waves propagation in anisotropic dielectrics and formulate problems and assumptions which we are using in our method. As a class of dielectrics we will study homogeneous, non-dispersive anisotropic dielectrics. Classification of these dielectrics according to the crystal systems and dielectric permittivity tensor \( \mathbf{\mathcal{E}} \) is also given in Section 2. This classification includes groups with diagonal matrices \( \mathbf{\mathcal{E}} \) (containing cubic, hexagonal, tetragonal, trigonal and orthorhombic structures) and groups with arbitrary symmetric matrices \( \mathbf{\mathcal{E}} \) (containing monoclinic and triclinic structures). Section 3 describes the procedure of finding the exact solution of the formulated problem. After that in Section 4 we describe the symbolic algorithms which are based on the combination of matrix operations.
and give their MATLAB code. As a result of these calculations we bring the exact formulae of matrices which are the main components of Fourier images of problem solutions for the groups of dielectrics mentioned above. Section 5 contains a set of figures obtained by exact formulae of problem solutions. These figures show the dynamics of electric wave propagation in these types of dielectrics.

2. Mathematical model of electromagnetic waves in anisotropic dielectrics and problems set-up

2.1. Crystallographic structures of anisotropic dielectrics and their dielectric tensor structures

It is known from crystallography that in crystalline materials the constituent atoms are arranged in a regular repeating configuration. Examining the structure of the three dimensional array of atoms in a crystal, we can determine the smallest building block that by repeated replication in three dimensions can create the structure of the crystal. This *unit cell* may have one of seven basic shapes, such as cubic, hexagonal, tetragonal, trigonal, orthorhombic, monoclinic, triclinic. These symmetry properties tell how the cell can be reflected, rotated and inverted to produce the same special arrangements of atoms. For linear homogeneous non-dispersive anisotropic dielectrics the electric flux density $D$ and the electric field $E$ have the following connection $D = \varepsilon E$. The relation of the crystallographic structures of anisotropic dielectrics with the structure of their dielectric permittivity tensor $\varepsilon$ is presented by Table 1 (see Dieulesaint and Royer, 1980).

2.2. Time-dependent Maxwell’s system

The propagation of electromagnetic waves in homogeneous, non-dispersive, anisotropic dielectrics is described by the time-dependent Maxwell’s system with a matrix of dielectric permittivity. Let $x = (x_1, x_2, x_3)$ be a space variable from $\mathbb{R}^3$, $t$ be a time variable from $\mathbb{R}$, then Maxwell’s system is given by the following relations (Ramo et al., 1994):

$$
curl \mathbf{H} = \varepsilon \frac{\partial \mathbf{E}}{\partial t} + \mathbf{j},
$$

(1)

$$
curl \mathbf{E} = -\mu \frac{\partial \mathbf{H}}{\partial t},
$$

(2)

$$
\text{div}(\mu \mathbf{H}) = 0,
$$

(3)

$$
\text{div}(\varepsilon \mathbf{E}) = \rho,
$$

(4)

<table>
<thead>
<tr>
<th>Crystallographic structure of dielectrics</th>
<th>Dielectric tensor $\varepsilon$ structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cubic</td>
<td>$\varepsilon = \text{diag}(\varepsilon_{11}, \varepsilon_{11}, \varepsilon_{11})$, $\varepsilon_{11} &gt; 0$</td>
</tr>
<tr>
<td>Hexagonal, tetragonal and trigonal</td>
<td>$\varepsilon = \text{diag}(\varepsilon_{11}, \varepsilon_{11}, \varepsilon_{33})$, $\varepsilon_{11} &gt; 0$, $\varepsilon_{33} &gt; 0$</td>
</tr>
<tr>
<td>Orthorhombic</td>
<td>$\varepsilon = \text{diag}(\varepsilon_{11}, \varepsilon_{12}, \varepsilon_{33})$, $\varepsilon_{11} &gt; 0$, $\varepsilon_{33} &gt; 0$, $\varepsilon_{12} &gt; 0$</td>
</tr>
<tr>
<td>Monoclinic</td>
<td>$\varepsilon = \begin{pmatrix} \varepsilon_{11} &amp; \varepsilon_{12} &amp; 0 \ \varepsilon_{12} &amp; \varepsilon_{22} &amp; 0 \ 0 &amp; 0 &amp; \varepsilon_{33} \end{pmatrix}$, $\varepsilon_{11} &gt; 0$, $\varepsilon_{33} &gt; 0$, $\varepsilon_{11}\varepsilon_{22} - \varepsilon_{12}^2 &gt; 0$</td>
</tr>
<tr>
<td>Triclinic</td>
<td>$\varepsilon = \begin{pmatrix} \varepsilon_{11} &amp; \varepsilon_{12} &amp; \varepsilon_{13} \ \varepsilon_{12} &amp; \varepsilon_{22} &amp; \varepsilon_{23} \ \varepsilon_{13} &amp; \varepsilon_{23} &amp; \varepsilon_{33} \end{pmatrix}$, $\varepsilon$ is symmetric positive definite</td>
</tr>
</tbody>
</table>

Table 1

Crystal systems and dielectric permittivity tensor structures
where \( \mathbf{E} = (E_1, E_2, E_3) \), \( \mathbf{H} = (H_1, H_2, H_3) \) are electric and magnetic fields, \( E_k = E_k(x,t) \), \( H_k = H_k(x,t) \), \( k = 1, 2, 3 \); \( \mathbf{j} = (j_1, j_2, j_3) \) is the density of the electric current, \( j_k = j_k(x,t) \), \( k = 1, 2, 3 \); \( \mu \) is the magnetic permeability, \( \varepsilon \) is the dielectric permittivity, \( \rho \) is the density of electric charges. The operator \( \text{curl}_x \) and \( \text{div}_x \) are defined by

\[
\text{curl}_x \mathbf{E} = \left( \frac{\partial E_3}{\partial x_2} - \frac{\partial E_2}{\partial x_3}, \frac{\partial E_1}{\partial x_3} - \frac{\partial E_3}{\partial x_1}, \frac{\partial E_2}{\partial x_1} - \frac{\partial E_1}{\partial x_2} \right),
\]

\[
\text{div}_x \mathbf{E} = \frac{\partial E_1}{\partial x_1} + \frac{\partial E_2}{\partial x_2} + \frac{\partial E_3}{\partial x_3}.
\]

The conservation law of charges is given by (see, for example, Ramo et al. (1994))

\[
\frac{\partial \rho}{\partial t} + \text{div}_x \mathbf{j} = 0. \tag{5}
\]

### 2.3. Assumptions and problems set-up

We assume in this paper that \( \mu = 1 \) and \( \varepsilon = (\varepsilon_{ij})_{3 \times 3} \) is a symmetric positive definite matrix with constant elements. Moreover we suppose that

\[
\mathbf{E} = 0, \quad \mathbf{H} = 0, \quad \rho = 0, \quad \mathbf{j} = 0 \quad \text{for} \quad t \leq 0, \tag{6}
\]

this means there is no electric charges and currents at the time \( t \leq 0 \); electric and magnetic fields vanish for \( t \leq 0 \).

**Remark 1.** We note that Eq. (3) follows immediately from (2), and Eq. (4) can be obtained from (1), (5) and (6). So equalities (1), (2) and (5) with conditions (6) imply (3) and (4).

Let further \( \varepsilon \) and \( \mathbf{j} \) be given. The main problem here is to find \( \mathbf{E}, \mathbf{H} \) satisfying (1) and (2) and condition (6).

**Remark 2.** We note that \( \rho \) can be defined as a solution of the initial value problem for the ordinary differential Eq. (5) with respect to \( t \), subject to \( \rho|_{t=0} = 0 \). Here \( \text{div}_x \mathbf{j} \) is given.

Differentiating (1) with respect to \( t \) and using (2) and (6) we find

\[
-\text{curl}_x \text{curl}_x \mathbf{E} = \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \frac{\partial \mathbf{j}}{\partial t}, \quad x \in \mathbb{R}^3, \quad t \in \mathbb{R}, \tag{7}
\]

\[
\mathbf{E}|_{t=0} = 0. \tag{8}
\]

Therefore for the solution of the main problem first of all we have to find \( \mathbf{E}(x,t) \) satisfying (7) and (8) and after that we can find \( \mathbf{H}(x,t) \) satisfying (2) and the condition \( \mathbf{H}|_{t=0} = 0 \) if \( \mathbf{E}(x,t) \) is given.

### 3. Finding the exact solution of (7) and (8)

Let \( \tilde{\mathbf{E}}(v,t), \tilde{\mathbf{j}}(v,t) \) be the Fourier transform images of the electric field \( \mathbf{E}(x,t) \) and current \( \mathbf{j}(x,t) \) with respect to \( x = (x_1, x_2, x_3) \in \mathbb{R}^3 \), i.e.

\[
\tilde{\mathbf{E}}(v,t) = \mathcal{F}_x[\mathbf{E}](v,t), \quad \tilde{\mathbf{j}}(v,t) = \mathcal{F}_x[\mathbf{j}](v,t),
\]
where
\[
\mathcal{F}_x [E](v, t) = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} E(x, t) e^{ix} \, dx_1 \, dx_2 \, dx_3,
\]
\[
v = (v_1, v_2, v_3), \quad xv = x_1 v_1 + x_2 v_2 + x_3 v_3, \quad i^2 = -1.
\]
The problem (7) and (8) can be written in terms of the Fourier image \( \tilde{E}(v, t) \) as follows:
\[
\begin{align*}
&\mathcal{S} \frac{\partial^2 \tilde{E}}{\partial t^2} + \mathcal{S}(v) \tilde{E} = -\frac{\partial \tilde{I}}{\partial t}, \quad t \in R, \quad v \in R^3, \\
&\tilde{E} |_{t=0} = 0, \quad v \in R^3,
\end{align*}
\]}
where
\[
\mathcal{S}(v) = \begin{pmatrix}
  v_1^2 + v_2^2 & -v_1 v_2 & -v_1 v_3 \\
  -v_1 v_2 & v_1^2 + v_3^2 & -v_2 v_3 \\
  -v_1 v_3 & -v_2 v_3 & v_1^2 + v_2^2
\end{pmatrix}.
\]
The method of exact solution consists of several steps. In the first step, using the transfer matrix formalism for given \( \mathcal{S}(v) \) and the symmetric positive definite matrix \( \mathcal{F} \) we construct a non-singular matrix \( \mathcal{F} \) and a diagonal matrix \( D(v) \) with non-negative elements such that
\[
\begin{align*}
&\mathcal{F}^T(v) \mathcal{S}(v) \mathcal{F}(v) = \mathcal{I}, \\
&\mathcal{F}^T(v) \mathcal{S}(v) \mathcal{F}(v) = \mathcal{D}(v),
\end{align*}
\]
where \( \mathcal{I} \) is the identity matrix, \( \mathcal{F}^T(v) \) is the transposed matrix to \( \mathcal{F}(v) \).

In the second step we are looking for the solution of (7) and (8) in the form
\[
\tilde{E}(v, t) = \mathcal{F}(v) Y(v, t),
\]
where the matrix \( \mathcal{F}(v) \) is constructed in the first step and a vector function \( Y(v, t) \) is unknown. Substituting (14) into (9) and (10) we find
\[
\begin{align*}
&\mathcal{S} \frac{\partial^2 Y}{\partial t^2} + \mathcal{S}(v) \mathcal{F} Y = -\frac{\partial \tilde{I}}{\partial t}, \quad t \in R, \quad v \in R^3, \\
&Y(v, t) |_{t=0} = 0, \quad v \in R^3.
\end{align*}
\]
Multiplying (15) by \( \mathcal{F}^T(v) \) and using (12) and (13) we have
\[
\frac{\partial Y}{\partial t} + \mathcal{D}(v) Y = -\mathcal{F}^T(v) \frac{\partial \tilde{I}}{\partial t}, \quad t \in R, \quad v \in R^3.
\]
In the third step of the method, using the ordinary differential equations technique, see, for example, (Boyce and DiPrima, 1992), a solution of the initial value problem (16) and (17) is given by
\[
Y(v, t) = \text{column}(Y_1(v, t), Y_2(v, t), Y_3(v, t)),
\]
where for \( t < 0 \) the function \( Y_n(v, t) \) vanishes and for \( t \geq 0 \) is defined by
\[
\begin{align*}
&Y_n(v, t) = -\int_0^t \cos(\sqrt{d_n(v)(t - \tau)}) |\mathcal{F}^T(v)\tilde{J}(v, \tau)|_n d\tau, \quad \text{if } d_n(v) > 0, \\
&Y_n(v, t) = -\int_0^t |\mathcal{F}^T(v)\tilde{J}(v, \tau)|_n d\tau, \quad \text{if } d_n(v) = 0; \quad n = 1, 2, 3,
\end{align*}
\]
where \( d_n(v), n = 1, 2, 3 \) are elements of the matrix \( D(v) \); \( |\mathcal{F}^T(v)\tilde{J}(v, \tau)|_n \) is the \( n \)th component of the vector \( \mathcal{F}^T(v)\tilde{J}(v, \tau) \).
Using formulae (14), (18)–(20) and given matrices \( \mathcal{F}(v), \mathcal{F}^T(v), D(v) \) found in the first step we find the Fourier image of the electric field \( \tilde{\mathbf{E}}(v,t) \). In the last step the electric field \( \mathbf{E}(x,t) \) is determined by the inverse Fourier transform \( \tilde{\mathcal{F}}_v^{-1} \) of \( \tilde{\mathbf{E}}(v,t) \), i.e.

\[
\mathbf{E}(x,t) = \tilde{\mathcal{F}}_v^{-1}[\tilde{\mathbf{E}}](x,t),
\]

\[
\tilde{\mathcal{F}}_v^{-1}[\tilde{\mathbf{E}}](x,t) = \frac{1}{(2\pi)^3} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \tilde{\mathbf{E}}(v,t) e^{i\omega_1 \mathbf{d}_1} \, dv_1 \, dv_2 \, dv_3.
\]  

(21)

4. Matrix formalism and its symbolic implementation in MATLAB

Let us consider in details this matrix formalism and its computer implementation, which simultaneously transfer the symmetric positive definite matrix \( \mathcal{E} \) and the matrix \( \mathcal{F}(v) \) defined by (11) into the identity matrix and a diagonal matrix with non-negative elements, respectively. This matrix formalism is based on the following procedures of the matrix theory (see, for example, (Goldberg, 1992)): finding \( \mathcal{E}^{-1/2} \), constructing an orthogonal matrix \( \mathcal{P}(v) \) of eigenvectors of \( \mathcal{E}^{-1/2} \mathcal{F}(v) \mathcal{E}^{-1/2} \) and a diagonal matrix \( \mathcal{D}(v) \) of eigenvalues of \( \mathcal{E}^{-1/2} \mathcal{F}(v) \mathcal{E}^{-1/2} \). Section 4.1 describes main properties of \( \mathcal{E}^{-1/2} \) matrix and a procedure of finding \( \mathcal{E}^{-1/2} \) in MATLAB code. Section 4.2 describes constructing matrix \( \mathcal{F}(v) \) and its implementation by MATLAB.

4.1. Finding \( \mathcal{E}^{-1/2} \)

Let us consider a symmetric positive definite matrix \( \mathcal{E} \). Matrix \( \mathcal{F} \) such that \( \mathcal{F}^2 = \mathcal{E} \) is denoted as \( \mathcal{E}^{1/2} \). The inverse matrix to \( \mathcal{E}^{1/2} \) is denoted as \( \mathcal{E}^{-1/2} \), i.e. \( \mathcal{E}^{-1/2} = (\mathcal{E}^{1/2})^{-1} \). There are the following properties of \( \mathcal{E}^{-1/2} \):

\[
\mathcal{E}^{-1/2} = \mathcal{E}^{1/2}, \quad (\mathcal{E}^{-1/2})^{-1} = \mathcal{E}^{1/2}; \quad \mathcal{E}^{-1/2} \text{ is symmetric positive definite.}
\]

The procedure of finding \( \mathcal{E}^{-1/2} \) contains the following operations.

\( O1 \) Find three linear independent eigenvectors of \( \mathcal{E} \). From these eigenvectors form the matrix where each eigenvector is a column. This matrix is denoted by \( \mathcal{P} \).

\( O2 \) Find three eigenvalues of \( \mathcal{E} \). Form the diagonal matrix with these eigenvalues on diagonal. Denote this matrix as \( \mathcal{M} \), i.e. \( \mathcal{M} = \text{diag}(\mu_1, \mu_2, \mu_3) \), where \( \mu_1, \mu_2 \) and \( \mu_3 \) are eigenvalues of \( \mathcal{E} \).

**Remark 3.** Since \( \mathcal{E} \) is positive definite then all its eigenvalues \( \mu_1, \mu_2 \) and \( \mu_3 \) are real and positive.

\( O3 \) Calculate the square root of \( \mathcal{M} \) by the formula

\[
\mathcal{M}^{1/2} = \text{diag}(\sqrt{\mu_1}, \sqrt{\mu_2}, \sqrt{\mu_3}).
\]

\( O4 \) Find the matrix \( \mathcal{E}^{1/2} \) by the formula \( \mathcal{E}^{1/2} = \mathcal{P} \mathcal{M}^{1/2} \mathcal{P}^{-1} \), where \( \mathcal{P} \) is the matrix found by \( O1 \), \( \mathcal{P}^{-1} \) is the inverse to \( \mathcal{P} \), \( \mathcal{M}^{1/2} \) is the matrix defined by \( O3 \).

\( O5 \) Find the matrix \( \mathcal{E}^{-1/2} \) by means of the formula \( \mathcal{E}^{-1/2} = (\mathcal{E}^{1/2})^{-1} \), where \( (\mathcal{E}^{1/2})^{-1} \) is the inverse to \( \mathcal{E}^{1/2} \).

MATLAB commands of above mentioned matrix operations are listed below.

```
INPUT: Eps;
[EigVecEps, EigValEps] = eig(Eps);
P = EigVecEps;
PT = P';
M = EigValEps;
```
\[ M_h = \sqrt{M}; \]
\[ \text{SqrEps} = \mathbf{P} \ast \mathbf{M_h} \ast \mathbf{P}^T; \]
\[ \text{InvSrtEps} = \text{inv} \left( \text{SqrEps} \right); \]
\[ \text{OUTPUT: SqrEps, InvSrtEps}. \]

Here
\[ \text{Eps, SqrEps, InvSrtEps} \]
are \( \varepsilon, \varepsilon^{1/2}, \varepsilon^{-1/2} \) respectively.

As an illustration let us consider the result of finding matrices \( \varepsilon^{1/2} \) and \( \varepsilon^{-1/2} \) for several different variants of \( \varepsilon \).

- **Orthorhombic dielectrics.** Let \( \varepsilon = \text{diag}(\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}) \) with symbolic input data. Then

\[
\varepsilon^{1/2} = \text{diag}(\sqrt{\varepsilon_{11}}, \sqrt{\varepsilon_{22}}, \sqrt{\varepsilon_{33}}), \quad \varepsilon^{-1/2} = \text{diag} \left( \frac{1}{\sqrt{\varepsilon_{11}}}, \frac{1}{\sqrt{\varepsilon_{22}}}, \frac{1}{\sqrt{\varepsilon_{33}}} \right).
\]

- **Monoclinic dielectrics.** Let

\[
\varepsilon = \begin{pmatrix}
\varepsilon_{11} & \varepsilon_{12} & 0 \\
\varepsilon_{12} & \varepsilon_{22} & 0 \\
0 & 0 & \varepsilon_{33}
\end{pmatrix}.
\]

Then \( \varepsilon^{1/2} \) and \( \varepsilon^{-1/2} \) are found by MATLAB symbolic calculations as follows:

\[
\varepsilon^{1/2} = \begin{pmatrix}
\varepsilon_{11} & \varepsilon_{12} & 0 \\
\varepsilon_{12} & \varepsilon_{22} & 0 \\
0 & 0 & \varepsilon_{33}
\end{pmatrix}, \quad \varepsilon^{-1/2} = \begin{pmatrix}
h_{11} & h_{12} & 0 \\
h_{12} & h_{22} & 0 \\
0 & 0 & h_{33}
\end{pmatrix},
\]

where

\[
e_{11} = \frac{1}{4d} \left[ m_{22}(\varepsilon_{11} - \varepsilon_{22} + d) - m_{11}(\varepsilon_{11} - \varepsilon_{22} - d) \right], \quad e_{12} = \frac{e_{12}}{2d}(m_{22} - m_{11}),
\]
\[
e_{22} = \frac{1}{4d} \left[ m_{11}(\varepsilon_{11} - \varepsilon_{22} + d) - m_{22}(\varepsilon_{11} - \varepsilon_{22} - d) \right], \quad e_{33} = \sqrt{\varepsilon_{33}},
\]
\[
h_{11} = \frac{1}{m_{11}m_{22}d} \left[ m_{11}(\varepsilon_{11} - \varepsilon_{22} + d) - m_{22}(\varepsilon_{11} - \varepsilon_{22} - d) \right],
\]
\[
h_{12} = \frac{2e_{12}}{m_{11}m_{22}d}(m_{11} - m_{22}), \quad h_{33} = \frac{1}{\sqrt{\varepsilon_{33}}},
\]
\[
h_{22} = \frac{1}{m_{11}m_{22}d} \left[ m_{22}(\varepsilon_{11} - \varepsilon_{22} + d) - m_{11}(\varepsilon_{11} - \varepsilon_{22} - d) \right],
\]
\[
d = \sqrt{(e_{11} - e_{22})^2 + 4e_{12}^2}, \quad m_{11} = \sqrt{2(e_{11} + e_{22} - d)}, \quad m_{22} = \sqrt{2(e_{11} + e_{22} + d)}.
\]

- **Triclinic dielectrics.** For triclinic dielectrics the matrix \( \varepsilon \) may have any arbitrary values with the single restriction—it must be symmetric and positive definite. Let us take numerical values like

\[
\varepsilon = \begin{pmatrix}
30.7929 & -12.7337 & -14.3432 \\
-12.7337 & 5.51479 & 5.86982 \\
-14.3432 & 5.86982 & 6.74556
\end{pmatrix}, \quad (22)
\]
then $\varepsilon^{1/2}$ and $\varepsilon^{-1/2}$ are found by MATLAB as follows:

$$
\varepsilon^{1/2} = 
\begin{pmatrix}
4.76923 & -1.84615 & -2.15385 \\
-1.84615 & 1.23077 & 0.769231 \\
-2.15385 & 0.769231 & 1.23077 \\
\end{pmatrix},
$$

$$
\varepsilon^{-1/2} =
\begin{pmatrix}
1.5 & 1.0 & 2.0 \\
1.0 & 2.0 & 0.5 \\
2.0 & 0.5 & 4.0 \\
\end{pmatrix}.
$$

### 4.2. Constructing $\mathcal{D}(v), \mathcal{F}(v)$

Using the procedure described in Section 4.1 the matrix $\varepsilon^{-1/2}$ is found, if $\varepsilon$ is known. As a result of it the matrix $\varepsilon^{-1/2} \mathcal{F}(v) \varepsilon^{-1/2}$ may be found as well. The procedure of constructing matrices $\mathcal{D}(v), \mathcal{F}(v)$ satisfying (12) and (13) for given $\varepsilon$ and $\mathcal{F}(v)$ consists of the following operations.

(O6) Find three linear independent orthonormal eigenvectors of $\varepsilon^{-1/2} \mathcal{F}(v) \varepsilon^{-1/2}$. From these eigenvectors form the matrix where each eigenvector is a column. Denote this matrix by $Q$.

(O7) Find three eigenvalues of $\varepsilon^{-1/2} \mathcal{F}(v) \varepsilon^{-1/2}$. Form the diagonal matrix with these eigenvalues on diagonal. Denote this matrix as $D$, i.e. $D(v) = \text{diag}(d_1(v), d_2(v), d_3(v))$, where $d_1(v), d_2(v), d_3(v)$ are eigenvalues of $\varepsilon^{-1/2} \mathcal{F}(v) \varepsilon^{-1/2}$.

**Remark 4.** Since $\varepsilon^{-1/2} \mathcal{F}(v) \varepsilon^{-1/2}$ is positive semi-definite then all its eigenvalues $d_1(v), d_2(v), d_3(v)$ are real and non-negative.

(O8) Calculate the matrix $\mathcal{F}(v)$ by the formula

$$
\mathcal{F}(v) = \varepsilon^{-1/2} \mathcal{D}(v).
$$

(O9) Find the matrix $\mathcal{F}^T(v)$ as transpose to $\mathcal{F}(v)$.

MATLAB commands of constructing $\mathcal{D}(v), \mathcal{F}(v)$ are listed below.

```
INPUT: InvSrtEps , S;
A = simplify(InvSrtEps*S*InvSrtEps);
[EigVecA, EigValA] = eig(A);
D = simplify(EigValA);
Q = simplify(EigVecA);
Q(:,1) = Q(:,1) ./ sqrt(sum (Q(:,1).^2));
Q(:,2) = Q(:,2) ./ sqrt(sum (Q(:,2).^2));
Q(:,3) = Q(:,3) ./ sqrt(sum (Q(:,3).^2));
T = InvSrtEps * Q;
transT = T.^
OUTPUT: D, T, transT.
```

Here $\text{InvSrtEps}, D, T, \text{transT}$

are $\varepsilon^{-1/2}$, $\mathcal{D}(v)$, $\mathcal{F}(v)$, $\mathcal{F}^T(v)$, respectively.

As an illustration let us demonstrate the result of constructing matrices $\mathcal{D}(v), \mathcal{F}(v)$ for different dielectrics.

- Orthorhombic dielectrics. The matrices $\mathcal{D}(v)$, and $\mathcal{F}(v)$ are found by MATLAB symbolic calculations as follows
\[ D(v) = \text{diag}(d_1(v), d_2(v), d_3(v)), \]
\[ F(v) = \begin{pmatrix}
T_{11}(v) & T_{12}(v) & T_{13}(v) \\
T_{21}(v) & T_{22}(v) & T_{23}(v) \\
T_{31}(v) & T_{32}(v) & T_{33}(v)
\end{pmatrix}, \]
\[ \Gamma(v) = v_1^4(h_{22}^3 - h_{33}^3)^2 + v_2^4(h_{11}^3 - h_{22}^3)^2 + v_3^4(h_{11}^3 - h_{33}^3)^2 \\
+ 2v_1^2v_2^2(h_{11}^2 - h_{22}^2)(h_{33}^2 - h_{22}^2) + 2v_1^2v_3^2(h_{22}^2 - h_{11}^2)(h_{22}^2 - h_{33}^2) \\
+ 2v_2^2v_3^2(h_{11}^2 - h_{33}^2)(h_{11}^2 - h_{33}^2)^2 \]
\begin{equation}
\begin{aligned}
d_1(v) &= 0, \quad d_2(v) = \omega(v) + \frac{1}{2} \dot{\lambda}(v), \quad d_3(v) = \omega(v) - \frac{1}{2} \dot{\lambda}(v), \\
T_{j1}(v) &= v_jZ(v), \quad T_{j2}(v) = [R_j(v) + Q_j(v)][M(v) + N(v)]^{-1/2}, \\
T_{j3}(v) &= [R_j(v) - Q_j(v)][M(v) - N(v)]^{-1/2}, \quad j = 1, 2, 3.
\end{aligned}
\end{equation}

Here

\begin{equation}
\begin{aligned}
\omega(v) &= \frac{51}{4} v_1^2 + \frac{55}{4} v_2^2 + \frac{25}{4} v_3^2 - \frac{9}{2} v_1 v_2 - \frac{23}{2} v_1 v_3 - 5v_2 v_3, \\
\lambda(v) &= 325v_1^4 + 689v_2^4 + 85v_3^4 - 190v_1^3 v_2 - 870v_1^3 v_3 - 226v_2^3 v_1 - 674v_2^3 v_3 \\
&\quad - 272v_3^3 v_1 - 374v_3^3 v_2 + 1100v_1^2 v_2^2 + 770v_1^2 v_3^2 + 658v_2^2 v_3^2 - 220v_1^2 v_2 v_3 \\
&\quad - 782v_2^2 v_1 v_3 + 504v_2^2 v_1 v_2, \\
Z(v) &= -\frac{13}{2} [1301v_1^2 + 233v_2^2 + 285v_3^2 - 1076v_1 v_2 - 1212v_1 v_3 + 496v_2 v_3]^{-1/2}, \\
Q_1(v) &= \frac{1}{2} [98v_1 - 48v_2 - 43v_3]Z_1(v), \\
Q_2(v) &= [74v_1 - 32v_2 - 33v_3]Z_1(v), \\
Q_3(v) &= \frac{1}{2} [79v_1 - 44v_2 - 34v_3]Z_1(v), \\
Z_1(v) &= [325v_1^4 + 698v_2^4 + 85v_3^4 - 190v_1^3 v_2 - 870v_1^3 v_3 - 226v_2^3 v_1 \\
&\quad - 674v_2^3 v_3 - 272v_3^3 v_1 - 374v_3^3 v_2 + 1100v_1^2 v_2^2 + 770v_1^2 v_3^2 \\
&\quad + 658v_2^2 v_3^2 - 220v_1^2 v_2 v_3 - 782v_2^2 v_1 v_3 + 504v_2^2 v_1 v_2]^{1/2}, \\
R_1(v) &= \frac{1}{2} [650v_1^3 - 388v_2^3 - 680v_3^3 - 2510v_1^2 v_2 - 1425v_1^2 v_3 + 1165v_2^2 v_3 \\
&\quad + 1471v_2^2 v_1 + 2021v_3^2 v_1 + 722v_3^2 v_2 - 1540v_1 v_2 v_3], \\
R_2(v) &= \frac{1}{2} [888v_2^3 - 1430v_1^3 - 255v_3^3 - 2363v_1^2 v_3 - 509v_2^2 v_2 - 1894v_2^2 v_1 \\
&\quad + 1550v_3^2 v_3 - 196v_3^2 v_1 + 53v_3^2 v_2 - 974v_1 v_2 v_3], \\
R_3(v) &= \frac{1}{2} [2665v_1^3 - 1676v_2^3 - 1224v_3^3 - 5139v_1^2 v_3 - 4973v_1 v_2 v_3 + 4837v_2^2 v_1 \\
&\quad + 1161v_2^2 v_3 + 4488v_3^2 v_1 + 1479v_3^2 v_2 - 2408v_1 v_2 v_3], \\
M(v) &= [718250v_1^6 + 290368v_2^6 + 37570v_3^6 - 1028300v_1^5 v_2 - 2564900v_1^5 v_3 \\
&\quad - 1400672v_1^4 v_3 - 300352v_1^3 v_2 - 94588v_2^4 v_2 - 288184v_2^4 v_3 \\
&\quad + 2921880v_1^4 v_3^2 + 3564470v_1^3 v_2^2 + 1788280v_1^3 v_3^2 + 21476v_2^3 v_2^3 \\
&\quad + 15028v_1^3 v_2^2 + 93964v_1^3 v_3^2 - 2637700v_1^2 v_2^3 - 2507180v_1^2 v_3^3 \\
&\quad - 4009980v_1^2 v_2^2 v_3 - 700700v_1^2 v_3^2 v_2 + 2423252v_1^2 v_3^2 v_2^2 + 1065662v_1^2 v_3^4 \\
&\quad + 1244620v_1 v_2^3 v_3 - 769860v_1 v_2^2 v_3^2 + 2679404v_1 v_2 v_3^3 \\
&\quad - 630864v_1 v_3^4 v_2 + 576368v_1 v_3^4 v_2 - 440804v_1 v_3^4 v_3^2 - 639548v_1 v_3^2 v_2^2].
\end{aligned}
\end{equation}
5. Images of the simulation of electric fields by (21)

We consider now examples of electric fields simulations obtained by the exact formula (21) for the solution of initial value problems for the time-dependent Maxwell’s system with different tensors of dielectric permittivity. For all these examples the current density $j$ was taken in the form

$$j(x, t) = e^1 \delta(x_1) \delta(x_2) \delta(x_3) \delta(t), \quad x = (x_1, x_2, x_3) \in \mathbb{R}^3,$$

where $e^1 = (1, 0, 0)$, $\delta(\cdot)$ is the Dirac delta function. This form of the current density is related to a directional pulse electric source concentrated at the origin of coordinates at the time $t = 0$ in the direction $e^1$. Results of the electric fields simulation are pictures of the first component of electric fields $E_1(x_1, x_2, x_3, t)$ obtained for $x_1 = 0$, or $x_2 = 0$, or $x_3 = 0$ for different time.

**Example 1 (Triclinic dielectric).** The matrix $\varepsilon$ is given by (22), $j(x, t)$ by (25). The result of the simulation $E_1(0, x_2, x_3, t)$ for $t = 0.01$ is presented in Fig. 1(a) and (b). The Fig. 1(a) is 3-D graph of $E_1(0, x_2, x_3, 0.01)$. On the vertical axis values of $E_1$ are plotted. The horizontal axes are $x_2, x_3$. The Fig. 1(b) is 2-D level plot of the same surface of $E_1(0, x_2, x_3, 0.01)$, i.e. the view of the surface $z = E_1(0, x_2, x_3, 0.01)$ from the top of $z$-axis.

Fig. 2 contains two screen shots of 2-D level plots of $E_1(0, x_2, x_3, 0.1)$, $E_1(x_1, x_2, 0, 0.1)$, respectively. The horizontal and vertical axes are $(x_2, x_3)$, $(x_1, x_2)$, respectively. There are several geometrical objects in Fig. 2(a) and (b). The object in the center of each picture has the complex configuration, several other objects around of the center look like ellipses.

**Example 2 (Monoclinic dielectric).** The matrix $\varepsilon$ is given by the following formula:

$$\varepsilon = \begin{pmatrix} 17.1598 & 13.0178 & 0 \\ 13.0178 & 23.6686 & 0 \\ 0 & 0 & 44.4444 \end{pmatrix}.$$

The results of the simulation of the electric wave propagation in this monoclinic dielectric are presented in Fig. 3.

Fig. 3(a) and (b) illustrate the dynamic of $E_1(0, x_2, x_3, t)$. Fig. 3(c) represents the image of $E_1(x_1, 0, x_3, 4)$ and Fig. 3(d) shows the image of $E_1(x_1, x_2, 0, 5)$.
Fig. 2. 2-D level plots of $E_1$ for triclinic dielectric. (a) $E_1(0, x_2, x_3, 0.1)$. (b) $E_1(x_1, x_2, 0, 0.1)$.

Fig. 3. 2-D level plots of $E_1$ for monoclinic dielectric. (a) $E_1(0, x_2, x_3, 3)$. (b) $E_1(0, x_2, x_3, 5)$. (c) $E_1(x_1, 0, x_3, 4)$ and (d) $E_1(x_1, x_2, 0, 5)$. 
Fig. 4. 2-D level plots of $E_1$ for orthorhombic dielectric. (a) $E_1(0, x_2, x_3, 7)$, (b) $E_1(0, x_2, x_3, 10)$, (c) $E_1(x_1, 0, x_3, 7)$, (d) $E_1(x_1, 0, x_3, 9)$, (e) $E_1(x_1, x_2, 0, 7)$ and (f) $E_1(x_1, x_2, 0, 11.5)$. 
Example 3 (Orthorhombic dielectric (magnesium niobate)). The diagonal matrix of the electric permittivity is given by

$$
\mathbf{\varepsilon} = \text{diag}(16.4, 20.9, 32.4).
$$

Two level plots of the following pairs $E_1(0, x_2, x_3, 7)$, $E_1(0, x_2, x_3, 10)$, and $E_1(x_1, 0, x_3, 7)$, $E_1(x_1, 0, x_3, 9)$, $E_1(x_1, x_2, 0, 7)$, $E_1(x_1, x_2, 0, 11.5)$ are presented in Fig. 4. In Fig. 4(a) there is a circle. Inside of this circle there is a set of circles and ellipses with the same center. In Fig. 4(b) we can see how these circles and ellipses are progressing. Fig. 4(c) contains an ellipse inside of which there is a set of circles with the same center. The dynamics of the wave propagation is shown in Fig. 4(d). The dynamics of $E_1(x_1, x_2, 0, t)$ is given in Fig. 4(e) and (f).

Example 4 (Hexagonal dielectric). The diagonal matrix of electric permittivity has two equal elements and this matrix is given by

$$
\mathbf{\varepsilon} = \text{diag}(11.1111, 11.1111, 44.4444).
$$

2-D level plots of $E_1(0, x_2, x_3, 6)$, $E_1(x_1, 0, x_3, 6)$, $E_1(x_1, x_2, 0, 6)$ are presented in Fig. 5.
Example 5 (*Cubic dielectric*). The diagonal matrix of the electric permittivity has three equal elements \( \varepsilon = \text{diag}(\varepsilon_{11}, \varepsilon_{11}, \varepsilon_{11}) \). In this case 2-D level plots of \( E_1(0, x_2, x_3, t) \), \( E_1(x_1, 0, x_3, t) \), \( E_1(x_1, x_2, 0, t) \) are presented by circles with the same radius for any fixed \( t \). We omit these figures because they are obvious.

6. Conclusions

In the paper we describe the efficient method for modeling electromagnetic wave propagations in homogeneous anisotropic dielectrics. This method is based on constructing an exact solution of the initial value problem by matrix symbolic calculations and the inverse Fourier transform which is done numerically. We note that the simulation of the wave phenomena based on exact solutions of initial value and initial boundary value problems for partial differential equations is the best one. The robustness of our approach is based on the modern achievements of computation algebra which allows us to make symbolic transformations of cumbersome formulae and matrices.

Using this approach we create a collection of images of electromagnetic wave fields and wave propagation for different types of dielectrics. This collection of images is organized now as a library which contains several hundreds of images which are classified according to crystal system. This library can be used as a set of patterns for study and development of anisotropic materials. At the same time it can be used for testing new numerical methods.

As a future application we plan to implement the library as a Web application and use media streaming technology to have access to the images from Internet.

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References