PML and PSTD Algorithm for Arbitrary Lossy Anisotropic Media

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Abstract—A general perfectly matched layer (PML) formulation is presented for lossy anisotropic media with arbitrary permittivity, permeability, and conductivity tensors. This PML is then used in a pseudospectral time-domain (PSTD) algorithm for solutions of electromagnetic fields in lossy anisotropic media. Numerical results verify the efficiency of the PML absorbing boundary condition and the PSTD algorithm.

Index Terms—Anisotropic media, pseudospectral time-domain (PSTD) method, time-domain analysis.

I. INTRODUCTION

BENNINGER’S perfectly matched layer (PML) [1] has become one of the best absorbing boundary conditions (ABC’s) for finite-difference time-domain (FDTD) and finite-element methods. It has been used in many applications involving isotropic and conductive media and in diagonally anisotropic media [2]–[4]. Recently, the extension of the PML formulations to more general anisotropic media has received considerable attention [5]–[7].

For the time-domain solutions in anisotropic media, one convenient approach (the material-independent PML (MIPML) [6]) for the PML formulation is to develop the absorber for vectors \( \mathbf{E} \) and \( \mathbf{H} \), recognizing that these vectors are more natural than \( \mathbf{E}_\perp \) and \( \mathbf{H}_\perp \) for anisotropic media. The formulation with \( \mathbf{E} \) and \( \mathbf{H} \) can become very difficult [5]. An elegant idea of the analytic continuation of partial differential equations to a complex variable spatial domain [8], [9] provides a straightforward way to formulate PML for anisotropic media. Recently, this method has been used to formulate the frequency-domain closed-form PML constitutive tensors for bianisotropic and dispersive media [7]. The formulation in [7] is Maxwellian and is particularly advantageous for finite-element methods in the frequency domain.

The objective of this work is twofold: 1) we extend the method of analytic continuation [9] to formulate the PML for lossy anisotropic media with arbitrary permittivity, permeability, and conductivity tensors \( \epsilon(\mathbf{r}) \), \( \mu(\mathbf{r}) \), and \( \sigma(\mathbf{r}) \) and 2) we develop a pseudospectral time-domain (PSTD) algorithm for field solutions in these arbitrary anisotropic media. In the conventional FDTD method for anisotropic media, it becomes necessary to interpolate field components over the Yee grid since all components are needed at any field location [10]. This requirement is avoided in the PSTD algorithm [11] since it uses a centered grid. Three-dimensional (3-D) numerical results for media with large anisotropy confirm the efficiency of the PML and the PSTD algorithm.

II. FORMULATION

A. PML for a Lossy Anisotropic Medium

Consider an inhomogeneous lossy anisotropic medium with space-dependent permittivity tensor \( \epsilon(\mathbf{r}) \), permeability tensor \( \mu(\mathbf{r}) \), and conductivity tensor \( \sigma(\mathbf{r}) \). The frequency-domain Maxwell’s curl equations are
\[
\nabla \times \mathbf{E} = i\omega \mathbf{B} - \mathbf{M}, \quad \nabla \times \mathbf{H} = -i\omega \mathbf{D} + \mathbf{J},
\]
where \( \mathbf{J} \) and \( \mathbf{M} \) are the imposed electric and magnetic current densities, respectively, and the constitutive relations are
\[
\mathbf{D} = \epsilon \mathbf{E}, \quad \mathbf{B} = \mu \mathbf{H}.
\]

To formulate the PML equations using the analytic continuation [9], the coordinate variable \( \eta (\eta = x, y, z) \) is replaced by a complex coordinate variable \( \hat{\eta} \) such that
\[
\hat{\eta} = \int_0^\eta \epsilon_\eta(\eta') d\eta', \quad \epsilon_\eta = \epsilon_0 + \frac{i\omega \eta}{\eta}
\]
where \( \exp(-i\omega t) \) time convention is used, and the real variables \( \epsilon_0 \) and \( \omega_0 \) are the PML scaling and attenuation coefficients, respectively. With the help of (3), the second equation of (1) can be rewritten as
\[
\frac{1}{c_\eta} \frac{\partial}{\partial \hat{\eta}} (\hat{\eta} \times \mathbf{H}) = -i\omega \mathbf{D} + \mathbf{J}.
\]

If we split the field \( \mathbf{D} \) into six scalar components \( D^{(\eta)}_\xi \) (\( \eta, \xi = x, y, z \) but \( \xi \neq \eta \))
\[
\mathbf{D} = \sum_{\eta=x,y,z} D^{(\eta)}_\eta = \sum_{\xi=x,y,z} \sum_{\xi \neq \eta \eta} \xi D^{(\eta)}_\xi
\]
(4) can be simplified by using (3) as
\[
\frac{\partial}{\partial \hat{\eta}} (\hat{\eta} \times \mathbf{H}) = -(i\omega \epsilon_\eta - \omega_\eta) D^{(\eta)} + \mathbf{J}^{(\eta)}
\]
where \( \mathbf{J}^{(\eta)} \) is the split electric current source. A similar split equation can be obtained for the first equation of (1).
The time-domain equations can be easily obtained from these split equations by Fourier transform:

\[
\frac{\partial}{\partial \eta} \bar{\eta} \times \bar{E} = -\frac{\partial}{\partial \eta} \left( \mathcal{B}^{(\eta)} \right) - \omega \mathcal{B}^{(\eta)} - \mathcal{M}^{(\eta)} \tag{7}
\]

\[
\frac{\partial}{\partial \eta} \bar{\eta} \times \bar{H} = a_{\eta} \frac{\partial}{\partial \eta} \left( \mathcal{D}^{(\eta)} \right) + \omega \left( \mathcal{B}^{(\eta)} + \mathcal{J}^{(\eta)} \right). \tag{8}
\]

These two equations are combined with the time-domain constitutive relations

\[
\mathcal{D} = \bar{\varepsilon} \bar{E} + \bar{\sigma} \int_{-\infty}^{t} \bar{E}(\tau) d\tau \quad \mathcal{B} = \bar{\mu} \bar{H} \tag{9}
\]

to obtain the solutions for \(\mathcal{E}, \mathcal{H}, \mathcal{D},\) and \(\mathcal{B}\). Note that \(\mathcal{E}\) and \(\mathcal{H}\) are the total fields and do not require a splitting. The FDTD and pseudospectral time-domain (PSTD) methods can then be utilized to solve (7)–(9).

### B. The PSTD Algorithm

Let us first consider the time integration of partial differential equations (7) and (8) together with (9). If \(\mathcal{D}\) and \(\mathcal{E}\) are sampled at \(t = n\Delta t\), and if \(\mathcal{B}\) and \(\mathcal{H}\) are sampled at \(t = (n+1/2)\Delta t\) where \(n\) is an integer, using the central time differencing scheme in (7) and (8) yields

\[
\mathcal{B}^{(n)}(n+1/2) = \frac{b_{\eta}}{d_{\eta}} \mathcal{B}^{(n)}(n-1/2) - \frac{1}{d_{\eta}} \mathcal{L}_{\eta}(\bar{\xi} \times \mathcal{E}) - \frac{1}{d_{\eta}} \mathcal{M}^{(n)} \tag{10}
\]

\[
\mathcal{D}^{(n)}(n+1) = \frac{b_{\eta}}{d_{\eta}} \mathcal{D}^{(n)}(n) + \frac{1}{d_{\eta}} \mathcal{L}_{\eta}(\bar{\xi} \times \mathcal{H}) - \frac{1}{d_{\eta}} \mathcal{J}^{(n)} \tag{11}
\]

where \(b_{\eta} = a_{\eta}/\Delta t - \omega /2\) and \(d_{\eta} = a_{\eta}/\Delta t + \omega /2\), and \(\mathcal{L}_{\eta} = \partial /\partial \eta\). These two equations give the explicit time-stepping formulas for updating the split fields from the previous time step. The total fields are then obtained from the constitutive relations (9) which, also after central time differencing, relate \(\mathcal{E}\) and \(\mathcal{H}\) to \(\mathcal{D}\) and \(\mathcal{B}\)

\[
\mathcal{E}(n+1) = \left( \bar{\varepsilon} + \frac{3}{2} \Delta t \bar{\sigma} \right)^{-1} \left[ \mathcal{D}(n+1) - \mathcal{D}(n) + \left( \bar{\varepsilon} - \frac{3}{2} \Delta t \bar{\sigma} \right) \mathcal{E}(n) \right] \tag{12}
\]

\[
\mathcal{H}(n+1/2) = \bar{\mu}^{-1} \mathcal{B}(n+1/2) \tag{13}
\]

where \(\mathcal{D}\) and \(\mathcal{B}\) are the total fields defined as in (5).

The difference between the FDTD and PSTD methods lies in the approximation of the spatial derivative operator \(\mathcal{L}_{\eta}\). In the FDTD method with a conventional staggered Yee grid, because of the nondiagonal nature of \(\bar{\varepsilon}, \bar{\mu},\) and \(\bar{\sigma},\) the interpolation of fields is required, as detailed by [10]. This interpolation decreases the FDTD accuracy, as the cell size \((\Delta x)\) is effectively doubled. With a centered grid where all field components are located at the cell center, the PSTD algorithm [11] avoids this interpolation. Furthermore, the PSTD algorithm provides a much higher order of accuracy for spatial derivatives, as described in [11].

In the PSTD algorithm, the spatial derivative \(\mathcal{L}_{\eta}\) is approximated by the fast Fourier transform (FFT) as

\[
\mathcal{L}_{\eta}\{f(\eta)\} \approx \mathcal{F}^{-1}\{ik_{\eta} \mathcal{F}\{f(\eta)\}\} \tag{14}
\]

where \(\mathcal{F}\) and \(\mathcal{F}^{-1}\) denote the forward and inverse FFT’s, and \(k_{\eta}\) is the Fourier variable in \(\eta\) direction. The representation in (14) is exact up to the Nyquist sampling rate, i.e., two cells per minimum wavelength. Therefore, there is no degradation of accuracy compared to the isotropic case.

### III. Numerical Results

Three-dimensional PSTD results are shown here for media with large anisotropy. The source has a Blackman–Harris window time function with a center frequency of \(f_{c} = 100\) MHz, and the discretization is \(\Delta x = \Delta y = \Delta z = 0.3\) m, \(\Delta t = 80\) ps. The first example shows the PML performance. It compares a \(32 \times 32 \times 32\) case with a much larger reference case to obtain the reflection from the PML absorbing boundary. The homogeneous lossy anisotropic medium has the following material properties:

\[
\begin{array}{ccc}
\bar{\varepsilon} &=& \begin{bmatrix} 1.75 & 0.433 & 0 \\ 0.433 & 1.25 & 0 \\
0 & 0 & 4 \end{bmatrix} \\
\bar{\mu} &=& \begin{bmatrix} 1.5 & 0.866 & 0 \\
0.866 & 0.5 & 0 \\
0 & 0 & 4 \end{bmatrix} \text{ S/m} \\
\bar{\eta} &=& \begin{bmatrix} 1.25 & 0.433 & 0 \\
0.433 & 1.75 & 0 \\
0 & 0 & 1.5 \end{bmatrix} 
\end{array}
\]
Ten PML cells with a linear profile $\alpha_{n} = 1$, $\omega_{n,\text{max}} = 1.6\pi f_{c}$ are used in each edge. The source is an $\hat{y}$-oriented electric dipole located at $(16, 16, 16)$, and two receiver arrays are: 1) the $y$ line receivers at locations $(18, j, 18)$ and 2) the $z$ line receivers at locations $(18, 18, j)$ where $j = 0, \cdots, 31$.

The comparison of the results with the reference results at $n = 300$ in Fig. 1(a) displays excellent agreement between the two results in the non-PML region of interest. The local reflection in Fig. 1(b) shows that the maximum reflection is below -60 dB.

In the second example we study the propagation of EM waves in an electrically anisotropic medium with the same $\hat{\varepsilon}$ tensor as in the last example, but isotropic $\hat{\mu} = \mu_{0}\hat{I}$ and $\hat{\sigma} = 0$.

An electric dipole in $y$ direction is located at $(16, 16, 16)$ in a grid of $128 \times 128 \times 128$, and an array of receivers are located along the $z$ direction at $(16, 16, 31 + [j - 1]5)$ where $j = 1, \cdots, 18$. Fig. 2 shows the received $E_{y}$ component. Clearly, two types of waves are excited which propagate in $z$ direction with the apparent velocities of $v_{x} = 1/\sqrt{\mu_{0}\varepsilon_{1}}$ and $v_{y} = 1/\sqrt{\mu_{0}\varepsilon_{2}}$, where $(\varepsilon_{1}, \varepsilon_{2}, \varepsilon_{3}) = (2, 1, 4)\varepsilon_{0}$ are the principal (diagonal) components of the $\hat{\varepsilon}$ tensor.

IV. CONCLUSIONS

The PML formulation for a lossy anisotropic medium with arbitrary permittivity, permeability, and conductivity tensors are presented using the idea of analytic continuation. A pseudospectral time-domain algorithm is developed to improve the accuracy of time-domain solutions of Maxwell’s equations in arbitrary anisotropic media and to avoid the interpolation of field components in the FDTD methods. The PML and PSTD formulation can also be easily extended to lossy bianisotropic media.

REFERENCES


