Analysis of Periodic Structures with Dispersive Material Using the FDTD Technique

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Abstract

A dispersive periodic boundary condition (DPBC) is developed for the finite-difference time-domain method to analyze periodic structures with dispersive media on the boundaries of a unit cell. The formulation is based on the auxiliary differential equation (ADE) with two-term Debye model and the constant horizontal wavenumber approach. The developed formulation is easy to implement and is efficient in both memory usage and computational time. The validity of this formulation is verified through a numerical example of an infinite dispersive slab.

1. Introduction

Periodic structures are of great importance in electromagnetics due to their wide range of applications. The finite-difference time-domain (FDTD) technique has been utilized to analyze these structures, and various periodic boundary conditions (PBC) have been developed such that the computations are performed on only one unit cell instead of the entire structure [1]. Electromagnetic simulation of dispersive media is essential in many applications such as medical telemetries, metamaterials designs, nanoplasmonic solar cells, shielding materials, etc. FDTD also provides an efficient means to simulate these media; various methods including the auxiliary differential equation (ADE) method [2] have been developed to model the frequency dependence of the material parameters in the FDTD simulations.

It's worthwhile to point out that most previous PBCs for FDTD technique are developed to analyze periodic structures where dispersive materials aren't located on the boundary of the unit cells. However, there are numerous applications where periodic structures with dispersive media on the boundaries of the unit cell exist. In this paper, a dispersive periodic boundary condition (DPBC) for FDTD technique is developed to solve the above challenge. The algorithm is based on the ADE technique with two-term Debye relaxation equation to simulate the general dispersive property in the medium. In addition, the constant horizontal wavenumber approach [3]-[4] is modified accordingly to implement the PBCs. The algorithm offers many advantages such as: computational efficiency, implementation simplicity, same stability condition and numerical errors as the conventional FDTD. The paper is organized as follows: In Section 2, brief descriptions of the ADE technique and the constant horizontal wavenumber approach are provided, FDTD updating equations are derived and the DPBC is described. In Section 3, a numerical example proving the validity of the approach is presented. Section 4 provides the conclusion.

2. The FDTD/DPBC Algorithm

In this section an algorithm to implement the DPBC in FDTD is developed. The algorithm is based on the ADE and the constant horizontal wavenumber approaches.

2.1 Auxiliary Differential Equation Approach

In the ADE method an additional differential equation relating the electric displacement vector $\boldsymbol{D}$ to the electric field vector $\boldsymbol{E}$ is used in addition to Maxwell's equations. For dispersive material the electric displacement vector can be written as:

$$\vec{D}(\omega) = \varepsilon(\omega)\vec{E}(\omega), \tag{1}$$

where ε is the permittivity of the medium. The dispersive characteristics of $\varepsilon(\omega)$ can be described by a two-term Debye relaxation equation as:

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$$\varepsilon(\omega) = \varepsilon_o \left[\varepsilon_\infty + \frac{\varepsilon_{s1} - \varepsilon_\infty}{1 + j\omega\tau_1} + \frac{\varepsilon_{s2} - \varepsilon_\infty}{1 + j\omega\tau_2} \right], \tag{2}$$

where ε_o is the free space permittivity, ε_s is the static or zero frequency relative permittivity, ε_∞ is the relative permittivity at infinite frequency and τ is the relaxation time. From (1) and (2) $\vec{D}(\omega)$ can be written as follows:

$$\vec{D}(\omega) = \varepsilon_o \frac{\varepsilon_s + j\omega(\varepsilon_{s1}\tau_2 + \varepsilon_{s2}\tau_1) - \omega^2\tau_1\tau_2\varepsilon_\infty}{1 + j\omega(\tau_1 + \tau_2) - \omega^2\tau_1\tau_2} \vec{E}(\omega), \tag{3}$$

where $\varepsilon_s = \varepsilon_{s1} + \varepsilon_{s2} - \varepsilon_\infty$. For time harmonic fields, equation (3) can be re-written into the differential time domain form as follows:

$$\tau_1\tau_2 \frac{\partial^2 \vec{D}(t)}{\partial t^2} + (\tau_1 + \tau_2)\frac{\partial \vec{D}(t)}{\partial t} + \vec{D}(t) = \varepsilon_o\varepsilon_s\vec{E}(t) + \varepsilon_o(\varepsilon_{s1}\tau_2 + \varepsilon_{s2}\tau_1)\frac{\partial \vec{E}(t)}{\partial t} + \tau_1\tau_2\varepsilon_o\varepsilon_\infty \frac{\partial^2 \vec{E}(t)}{\partial t^2}. \tag{4}$$

Now following the FDTD procedure, new H field components are updated based on current H and E field components, following that the new D field components are updated based on current D and H field components. The new E field components are then updated using equation (4) based on the new D field components, the previous and twice in time previous D field components, and the current and previous E field components [5].

2.2 Constant Horizontal Wavenumber Approach

For periodic structure with periodicity P_x along the x-direction the PBC of the electric field in frequency domain can be written according to Floquet theory as:

$$E(x = 0, y, z, \omega) = E(x = P_x, y, z, \omega) \times e^{jk_xP_x}, \tag{5}$$

where

$$k_x = k_0 \sin\theta = \frac{2\pi f}{c}\sin\theta, \tag{6}$$

and c is speed of light in free space. Instead of fixing the angle θ, the constant horizontal wavenumber approach fixes the value of the horizontal wavenumber k_x in the FDTD simulation. Thus, the term $e^{jk_xP_x}$ is considered constant in (5). Using direct frequency domain to time domain transformation, the field in time domain can be represented as follows:

$$E(x = 0, y, z, t) = E(x = P_x, y, z, t) \times e^{jk_xP_x}. \tag{7}$$

In this approach, conventional Yee's scheme is used to update the ***E*** and ***H*** field components which offer several advantages, such as implementation simplicity, same stability condition and numerical errors as conventional FDTD technique. In addition, this approach has good computational efficiency for near grazing incident angles [3]. This makes the constant horizontal wavenumber approach a good choice for the periodic structure analysis as outlined in [3,4].

2.3 Implementation of Dispersive Periodic Boundary Condition

The computational domain is shown in Fig. 1(a). The algorithm is based on the ADE technique to update the magnetic field components and the non-boundary electric field components. In addition, a modified version of the constant horizontal wavenumber approach is derived to update electric filed components on the boundaries. The algorithm can be summarized as follows:

1. Update ***H*** from ***E*** using conventional FDTD.
2. Update ***D*** from ***H*** (non-boundary components) using the ADE technique.
3. Update ***D*** from ***H*** (boundary components) using DPBC.
4. Update ***E*** from ***D*** using the ADE technique.

Steps 1, 2 and 4 don't need any further modification compared to the conventional FDTD and the ADE technique; only for step 3 the constant horizontal wavenumber approach should be modified. The Floquet theory in frequency domain is represented as follows:

$$E(x, y = 0, z, \omega) = E(x, y = P_y, z, \omega) \times e^{jk_yP_y}. \tag{8}$$

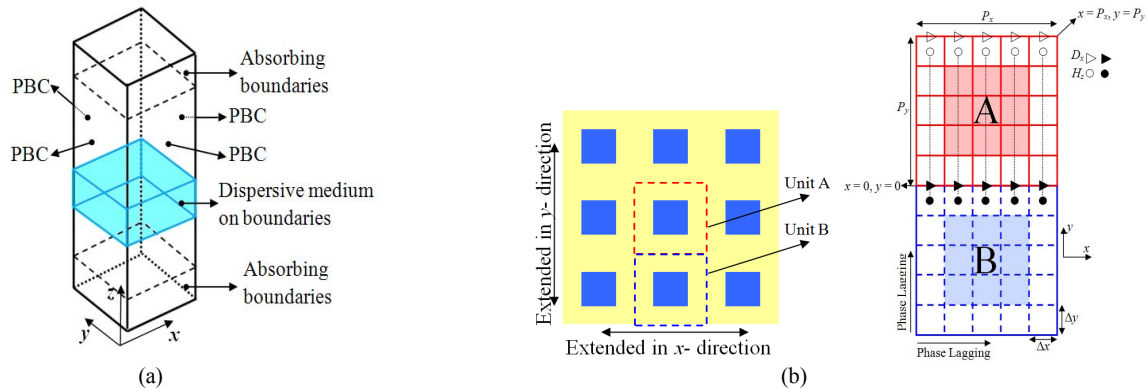


Fig. 1 (a) Computational domain (unit cell geometry), (b) Geometry of a general periodic structure.

Multiplying both sides of equation (8) by the complex permittivity will result in the following equation:

$$D(x, y = 0, z, \omega) = D(x, y = P_y, z, \omega) \times e^{jk_y P_y}. \tag{9}$$

Equation (9) represent Floquet theory for the displacement electric field vector $\boldsymbol{D}$. Using the constant horizontal wavenumber approach, equation (9) can be directly transformed to the time domain as follows:

$$D(x, y = 0, z, t) = D(x, y = P_y, z, t) \times e^{jk_y P_y}. \tag{10}$$

For the x-direction, the updating equation for the $\boldsymbol{D}$ components on the boundary can be written as follows for the boundary $y = 0$:

$$\begin{aligned} D_x^{n+1}(i,1,k) &= C_{dxd}(i,1,k) \times D_x^n(i,1,k) \\ &+ C_{dxhz}(i,1,k) \times [H_z^{n+\frac{1}{2}}(i,1,k) - H_z^{n+\frac{1}{2}}(i,0,k)] \\ &+ C_{dxhy}(i,1,k) \times [H_y^{n+\frac{1}{2}}(i,1,k) - H_y^{n+\frac{1}{2}}(i,1,k-1)]. \end{aligned} \tag{11}$$

From equation (11) it can be noticed that updating the $\boldsymbol{D}$ components on the boundary $y = 0$ need the knowledge of magnetic field components outside our unit cell of interest (unit A in Fig. 1(b)), but due to the periodicity and using the Floquet theory one can use magnetic field components H_z inside unit A to update these electric displacement fields as follows:

$$H_z^{n+\frac{1}{2}}(i,0,k) = H_z^{n+\frac{1}{2}}(i,n_y,k) \times e^{jk_y P_y}, \tag{12}$$

where n_y is the total number of FDTD cell in the y-direction. Using equation (11) and (12) all the displacement electric field components on the boundary $y = 0$ can be updated. As for the boundary $y = P_y$ the updating equation can be represented as follows:

$$D_x^{n+1}(i, n_y + 1, k) = D_x^{n+1}(i,1,k) \times e^{-jk_y P_y}. \tag{13}$$

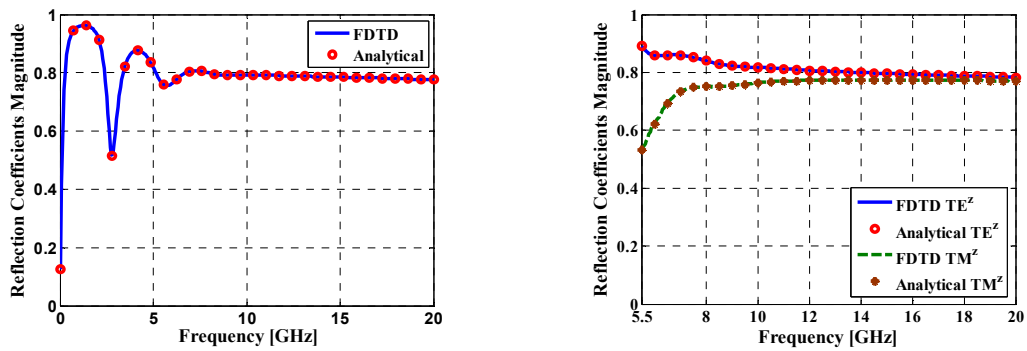
Similar to the approach for x-direction, all the fields in both y- and z- directions can be updated. In addition, the algorithm can be used for non-dispersive dielectric material by setting both τ_1 and τ_2 in equation (2) to zeros. The FDTD/DPBC algorithm can be easily extended to implement both frequency dependent permittivity and permeability media. In addition, the DPBC can be simply used with other dispersive models such as Lorentz or Drude model, and can be used with other dispersive simulation techniques such as recursive convolution and Z-transform.

3. Numerical Results

In this section, numerical results generated using the FDTD/DPBC algorithm are presented. The FDTD code was developed using MATLAB [6] on a personal computer with an Intel Core 2, 2.66GHz with 2 GB RAM. These results demonstrate the validity of the algorithm for determining scattering properties of periodic structures with general dispersive media. The results are compared with results obtained from an analytical solution.

The algorithm is used to analyze an infinite water slab with thickness 6 mm. The slab is illuminated by TM^z and TE^z plane waves in two different simulations. The parameters of water permittivity are obtained from [5] as: $\varepsilon_{s1} = 81$,

$\varepsilon_{s2} = 1.8$, $\varepsilon_\infty = 1.8$, $\tau_1 = 9.4 \times 10^{-12}$ and $\tau_2 = 0$. The geometry of the slab is shown in Fig. 1(a). The FDTD grid cell size is $\Delta x = \Delta y = \Delta z = 0.125$ mm, and the slab is represented by 2×2 cells (due to the homogeneity of the infinite slab it can be considered as a periodic structure with any periodicity). In the FDTD code 10,000 time steps are used. Convolutional Perfect Matched Layer (CPML) is used as the absorbing boundaries at the top and the bottom of the computational domain as implemented in [7]. The slab is excited using cosine modulated Gaussian pulse centered at 10 GHz and with 20 GHz bandwidth (bandwidth of modulated Gaussian pulse is defined as the frequency band where the magnitude of the frequency domain reaches 10% of its maximum) for the normal incident case ($k_x = 0$ m^{-1}), and it is excited using cosine modulated Gaussian pulse centered at 12.75 GHz and with 14.5 GHz bandwidth for the oblique incident case ($k_x = 104.8$ m^{-1}). The results are compared with analytical results. From Fig. 2 good agreements between analytical solutions and FDTD results can be noticed for both TM^z and TE^z cases (normal and oblique incidence).



(a) (b)

Fig. 2 Reflection coefficient for infinite water slab of thickness 6mm: (a) Under normal incidence ($k_x = 0$ m^{-1}), (b) Under TM^z and TE^z oblique incidence ($k_x = 104.8$ m^{-1}).

4. Conclusion

This paper introduces DPBC to analyze the scattering properties of periodic structures with dispersive media on the boundaries using FDTD. The approach is developed based on both the constant horizontal wavenumber technique and the ADE technique. It is simple to implement and is efficient in terms of both computational time and memory usage. The algorithm is capable of calculating the scattering parameters in case of normal and oblique incidence, for both TE^z and TM^z cases. Numerical example for a dispersive slab was provided, and the results show good agreement with results from the analytical solution.

5. References

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