Efficient Leapfrog SF FDTD Method for Periodic Structures at Oblique Incidence

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Abstract **─** This paper presents an efficient explicit leapfrog implementation of the split-field (SF) finite-difference time-domain (FDTD) method for solving problems of the oblique incident plane wave on periodic structures. Firstly, by splitting only one field component, the additional time derivative terms of transformed Maxwell's equations can be eliminated. Then, by applying Peaceman–Rachford scheme, one-step leapfrog scheme and Sherman-Morrison formula, the proposed SF method is implemented in a much simpler explicit scheme than traditional SF FDTD method and some unconditionally stable methods. Furthermore, the stability condition of the proposed method is weaker than traditional SF FDTD method. The accuracy and efficiency of this method are verified by numerical results.

Index Terms **─** Finite-difference time-domain (FDTD) algorithm, modified split-field (SF) method, one-step leapfrog scheme, periodic structure.

I. INTRODUCTION

Many electromagnetic applications possess a periodicity in one or more dimensions, such as dielectric frequency selective surfaces (DFSS) [1], photonic bandgap (PBG) structures [2] and so on. The analyses of these structures using the conventional finite-difference time-domain (FDTD) method are time-consuming and memory-extensive because the periodic structures exist. The periodic boundary condition (PBC) provides a good choice to alleviate the computational burden in analyzing these structures' scattering problems [3] because only one unit cell of the periodicity need to be modeled. However, PBC is difficult to implement at the oblique incident due to a cell-to-cell phase variation between two periodic boundaries [4]. The methods that have been proposed for oblique incident are divided into two main categories: direct field methods and field transformation methods [5]. The split-field (SF) FDTD method [4], which belongs to the second category, is widely used because it is very useful and robust. Unfortunately, the Courant Friedrichs Lewy (CFL) conditions of the SF FDTD method is strict and angle-dependent. To overcome the restriction, some unconditionally stable methods [6, 7] based on implicit scheme have been introduced into the analysis of periodic structures. However, those methods all need to solve several complex implicit equations and exhibit worse numerical dispersion errors along with the increment of the time-step size. After that, Wang *et al*. present an explicit implementation of the 2-D SF FDTD method [8] by locally one-dimensional (LOD) scheme.

In this paper, by adopting modified SF method [9], Peaceman–Rachford (PR) scheme [10] and one-step leapfrog scheme [11], an efficient explicit leapfrog SF FDTD method is proposed for analyzing the oblique incident plane wave problems in periodic structures. In comparisons with the traditional SF FDTD method [4] and LOD FDTD method [7], the proposed method has better numerical performance, which is validated by the numerical examples. The rest of this paper is arranged as follows, Section II presents the derivation of formulation. In Section III, the numerical performance of the proposed method is analyzed. In Section IV, two numerical examples are demonstrated to verify the computational accuracy, efficiency and memory storage of this method by comparing with traditional SF FDTD method and periodic LOD FDTD method [7], and the conclusions are drawn in Section V.

II. FORMULATION

Supposing that an electromagnetic object has a periodic structure in *y*-direction, according to field transformation technique [3, 5], the transformed Maxwell's equations for 2-D TM wave can be obtained as follows:

$$\frac{\mu_r}{c}\frac{\partial Q_x}{\partial t} = -\frac{\partial P_z}{\partial y} + \frac{\sin\theta}{c}\frac{\partial P_z}{\partial t}, \qquad (1)$$

$$\frac{\mu_r}{c}\frac{\partial Q_y}{\partial t} = \frac{\partial P_z}{\partial x}, \qquad (2)$$

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$$\frac{\varepsilon_r}{c}\frac{\partial P_z}{\partial t}=\frac{\partial Q_y}{\partial x}-\frac{\partial Q_x}{\partial y}+\frac{\sin\theta}{c}\frac{\partial Q_x}{\partial t}\,, \tag{3}$$

where $Q_x=\eta_0 H_x e^{jk_y y}$, $Q_y=\eta_0 H_y e^{jk_y y}$, $P_z=E_z e^{jk_y y}$ and $k_y=\omega\sin\theta/c$. c is the speed of light in free space, θ is the angle of propagation for the incident field, ε_r and μ_r are relative permittivity and relative permeability, respectively.

It can be seen from equations (1) and (3) that these equations cannot be implemented yet since the time derivative terms appear in both sides of equations.

In our early work [9], a new SF method is proposed to eliminate the additional time derivative terms of equations (1)-(3) as follows:

$$\frac{\partial Q_{xa}}{\partial t}=-a_1\frac{\partial P_z}{\partial y}\,, \tag{4}$$

$$\frac{\partial Q_y}{\partial t}=a_1\frac{\partial P_z}{\partial x}\,, \tag{5}$$

$$\frac{\partial P_z}{\partial t}=a_2\left(\frac{\partial Q_y}{\partial x}-\frac{\partial Q_{xa}}{\partial y}\right)-a_3\frac{\partial P_z}{\partial y}\,, \tag{6}$$

where $a_1=c/\mu_r$, $b_1=\varepsilon_r\mu_r-\sin^2\theta$, $a_2=c\mu_r/b_1$, $a_3=2c\sin\theta/b_1$.

Equations (4)-(6) are self-consistent, which is simpler than the traditional SF FDTD method that need to calculate two other fields (Q_{xa} and P_{za}).

By applying the PR scheme [10], equations (4)-(6) can be split into two sub-steps as:

(n)th-(n+1/2)th step:

$$Q_{xa}^{n+1/2}+a_1a_5\frac{\partial}{\partial y}P_z^{n+1/2}=Q_{xa}^{n}\,, \tag{7}$$

$$Q_{y}^{n+1/2}-a_1a_5\frac{\partial}{\partial x}P_z^{n+1/2}=Q_{y}^{n}\,, \tag{8}$$

$$\left(1+a_3a_5\frac{\partial}{\partial y}\right)P_z^{n+1/2}=a_5\left(-a_2\frac{\partial}{\partial y}Q_{xa}^{n}+a_2\frac{\partial}{\partial x}Q_{y}^{n}\right)+P_z^{n}\,. \tag{9}$$

(n+1/2)th-(n+1)th step:

$$Q_{xa}^{n+1}=Q_{xa}^{n+1/2}-a_1a_5\frac{\partial}{\partial y}P_z^{n+1/2}\,, \tag{10}$$

$$Q_{y}^{n+1}=Q_{y}^{n+1/2}+a_1a_5\frac{\partial}{\partial x}P_z^{n+1/2}\,, \tag{11}$$

$$a_5\left(a_2\frac{\partial}{\partial y}Q_{xa}^{n+1}-a_2\frac{\partial}{\partial x}Q_{y}^{n+1}\right)+P_z^{n+1}=\left(1-a_3a_5\frac{\partial}{\partial y}\right)P_z^{n+1/2}\,, \tag{12}$$

where $a_5=\Delta t/2$ and Δt is the time step size.

In order to achieve better computational efficiency, one-step leapfrog technique [11] is introduced into the proposed method. We suppose that P_z is updated at half time steps, while Q_{xa} and Q_y are updated at integer time steps.

By substituting equations (7) and (8) into (10) and (11) respectively, the updating equations for Q_{xa} and Q_y can be got easily:

$$Q_{xa}^{n+1}=Q_{xa}^{n}-\Delta t a_1\frac{\partial}{\partial y}P_z^{n+1/2}\,, \tag{13}$$

$$Q_{y}^{n+1}=Q_{y}^{n}+\Delta t a_1\frac{\partial}{\partial x}P_z^{n+1/2}\,. \tag{14}$$

Then, substitute equation (12) in the previous time step into equation (9), the updating equation for P_z is obtained as:

$$\begin{aligned}&\left(1+a_3a_5\frac{\partial}{\partial y}\right)P_z^{n+1/2}=\\&\Delta t\left(-a_2\frac{\partial}{\partial y}Q_{xa}^{n}+a_2\frac{\partial}{\partial x}Q_{y}^{n}\right)+\left(1-a_3a_5\frac{\partial}{\partial y}\right)P_z^{n-1/2}\end{aligned}\,. \tag{15}$$

To further simplify, an auxiliary field variable ρ_z is introduced as:

$$\rho_z^{n+1/2}=P_z^{n+1/2}+P_z^{n-1/2}\,. \tag{16}$$

Then, the (15) can be rewritten as:

$$\left(1+a_3a_5\frac{\partial}{\partial y}\right)\rho_z^{n+1/2}=\Delta t\left(-a_2\frac{\partial}{\partial y}Q_{xa}^{n}+a_2\frac{\partial}{\partial x}Q_{y}^{n}\right)+2P_z^{n-1/2}\,. \tag{17}$$

After that, the final implementation of the proposed leapfrog SF FDTD method is: equations (17)-(13)-(14). The field components are computed in a full time step like the conventional FDTD method, where no substep computations are needed. It means that the real iterative time step of the proposed method is Δt.

Updating $\rho_z^{n+1/2}$ from equation (17) with the PBC requires solving a perturbed bidiagonal system, which is:

$$G_1\rho_{z(i)}^{n+1/2}=d\,, \tag{18}$$

$$G_1=\begin{bmatrix}g_1 & & & & g_2\\ g_2 & g_1 & & & \\ & & \vdots & & \\ & & g_2 & g_1 & \\ & & & g_2 & g_1\end{bmatrix},\ \rho_{z(i)}=\begin{bmatrix}\rho_{z(i,2)}\\ \rho_{z(i,3)}\\ \vdots\\ \rho_{z(i,N_y-1)}\\ \rho_{z(i,N_y)}\end{bmatrix},\ d=\begin{bmatrix}d_{(i,2)}\\ d_{(i,3)}\\ \vdots\\ d_{(i,N_y-1)}\\ d_{(i,N_y)}\end{bmatrix},$$

where $g_1=1/2+a_3/\Delta y$, $g_2=1/2-a_3/\Delta y$, N_y is the maximum mesh number in y-direction. d is the right-hand-sides of equation (17), which is known.

To implement equation (18) explicitly, the Sherman-Morrison formula [12] can be applied as:

$$G_2p_a=d\,, \tag{19}$$

$$G_2p_b=w\,, \tag{20}$$

$$\rho_{z(i)}^{n+1/2}=p_a+\left(p_{a(i,N_y)}p_b\right)\left(1-p_{b(i,N_y)}\right)^{-1}\,, \tag{21}$$

where

$$G_2=G_1-wz=\begin{bmatrix}g_1 & & & & \\ g_2 & g_1 & & & \\ & & \vdots & & \\ & & g_2 & g_1 & \\ & & & g_2 & g_1\end{bmatrix}\,. \tag{22}$$

$$w=\begin{bmatrix}g_2 & 0 & \cdots & 0\end{bmatrix}^T,\ z=\begin{bmatrix}0 & 0 & \cdots & 1\end{bmatrix}$$

The perturbed bidiagonal system (equation (18)) is converted into two auxiliary linear systems (equations (19) and (20)) that can be solved explicitly.

Taking the equation (19) as an example:

$$p_{a(i,2)}=d_{(i,2)}/g_1\,, \tag{23}$$

$$p_{a(i,j)} = \left(d_{(i,j)} - g_2 p_{a(i,j-1)}\right) / g_1 \;\; 3 \le j \le N_y \,. \qquad (24)$$

The realization of equation (20) can be handled similarly as the above-mentioned approach for equation (19). With the solution of $\rho_z^{n+1/2}$, the field components $P_z^{n+1/2}$, Q_{xa}^{n+1} and Q_y^{n+1}can be calculated explicitly by using equations (16), (13) and (14), respectively.

III. NUMERICAL PERFORMANCE ANALYSIS

A. Numerical stability analysis

The CFL condition of the proposed method can be analyzed by the Fourier method [3, 12]. Assuming a plane wave propagating in the grid, the amplification factors in free space from (n)th to (n+1)th time step can be obtained as:

$$\lambda_1 = 1, \lambda_{2,3} = \left(-\nu_3 \pm i\sqrt{4\nu_1\nu_2 - \nu_3^2}\right)\Big/ 2\nu_1 \,, \qquad (25)$$

where $i=\sqrt{-1}$, $k_x=\omega\cos\theta/c$, $m_1=c\Delta t\sin(k_x\Delta x/2)/\Delta x$, $m_2=c\Delta t\sin(k_y\Delta y/2)/\Delta y$, $\upsilon_0=2im_2\sin\theta/\cos^2\theta$, $\upsilon_1=\upsilon_0-1$, $\upsilon_2=-\upsilon_0-1$ and $\upsilon_3=2(2(m_1^2+m_2^2)/\cos^2\theta-1)$.

To make the difference scheme to be stable, the magnitude of amplification factors should be less than or equal to unity. Therefore, the CFL stability condition can be derived as:

$$\Delta t \le \cos\theta \Big/ \left(c\sqrt{\Delta x^{-2} + \Delta y^{-2}}\right). \qquad (26)$$

In contrast, the stability condition of the traditional split-field FDTD method for square cell is $\Delta t \le \Delta x\cos^2\theta / c\sqrt{1+\cos^2\theta}$ [3], and its iterative time step is $\Delta t/2$. It can be seen easily that the stability condition of the proposed method is more relaxed, especially at the high incident angle.

B. Memory and computational efficiency analysis

Meanwhile, in terms of the memory used, the amount of the field components needs to be stored by the proposed method (p_a, $P_z^{n+1/2}$, $\rho_z^{n+1/2}$, Q_{xa}^n, Q_y^n) is similar to the LOD FDTD method and less than that of the traditional SF FDTD method ($Q_{xa}^{n-1/2}$, Q_{xa}^n, Q_x^n, $Q_y^{n-1/2}$, Q_y^n, $P_{za}^{n-1/2}$, P_{za}^n, P_z^n). In addition, it can be seen that the final implementation doesn't need to solve implicit equations, which is more efficient than those unconditionally stable methods [6, 7] because those methods all need to solve more than two complex implicit equations.

IV. NUMERICAL VALIDATION

For validating the accuracy and efficiency of the proposed method, the scattering properties of a PBG structure and a DFSS structure are presented, respectively.

In the first example, a PBG structure in Fig. 1 (same as [4, 7]) with four infinitely long dielectric rods is simulated. The computational domain is meshed by 308×38 uniform grids ($\Delta x=\Delta y$=0.25mm) and truncated by the PBC and the perfectly matched layer (PML) absorbing boundary condition along the y-direction and x-direction, respectively. A total-field/scattered-field (TF/SF) connecting boundary is applied to excite a plane wave and the total simulation time is chosen as 8.3 ns.

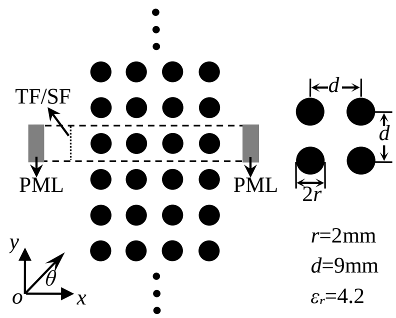


Fig. 1. Geometry of a photonic bandgap.

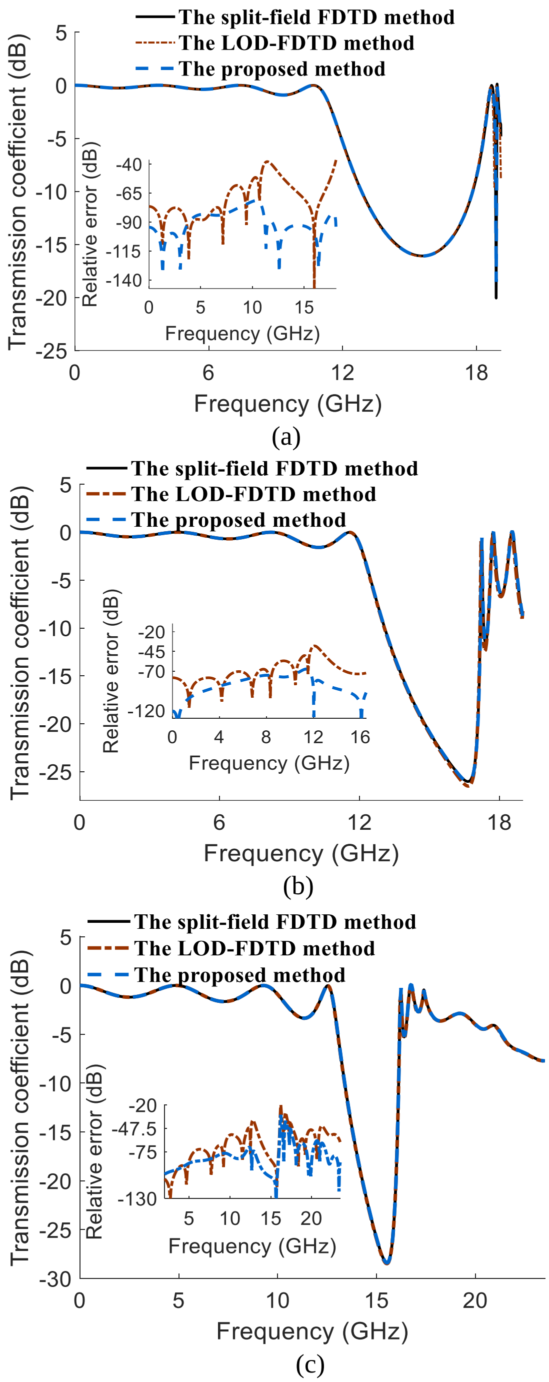
In this example, four different incident cases of (θ=30°, 45°, 60°and 75°) are calculated by the traditional SF FDTD method, the periodic LOD FDTD method [7] and the proposed method. The traditional SF FDTD method is used as the benchmark to examine the computational accuracy of other methods because its numerical dispersion error is the smallest. To achieve enough accuracy, the time-step sizes of the three methods are: t_1, 6×t_1 and CFLN×t_1, respectively. t_1 is half of the max time step size of traditional SF FDTD method from [3]. CFLN indicates the largest integer ratio maximum between the time-step size in proposed method from equation (26) and t_1.

The results of transmission coefficient and relative errors of the above-mentioned methods are plotted in Fig. 2. The information of the computational resources is listed in Table 1. Figure 2 shows that the numerical results calculated by the proposed method have a good agreement with traditional SF FDTD method (the relative error is below -45 dB), and the proposed method achieves better numerical dispersion performance than the LOD FDTD method. Table 1 manifests that the proposed method has high efficiency, especially at the high incident angle. Moreover, the memory storage of the proposed method is less than that of the other two methods from Table 1.

Table 1: CPU times and memory cost of the simulation of the first example

Method	**Memory (kB)**	**CPU Time (s) (CFLN)**			
		θ=30°	θ=45°	θ=60°	θ=75°
The traditional SF FDTD method	978	32.71	38.27	62.53	223.35
The LOD method	570	8.39 (6)	9.54 (6)	15.29 (6)	55.28 (6)
The proposed method	376	10.22 (2)	11.7 (2)	15.43 (3)	31.68 (5)

In the second example, to further validate the effectiveness, the proposed method is utilized to simulate the electromagnetic properties of a DFSS with two dielectric slabs (ε_{r1}=10, ε_{r2}=5) shown in Fig. 3. The computational domain is meshed by 200×20 uniform grids. The grid size, the time step size and the boundary conditions of the example are identical with the former. The total simulation time is chosen as 0.25 μs.



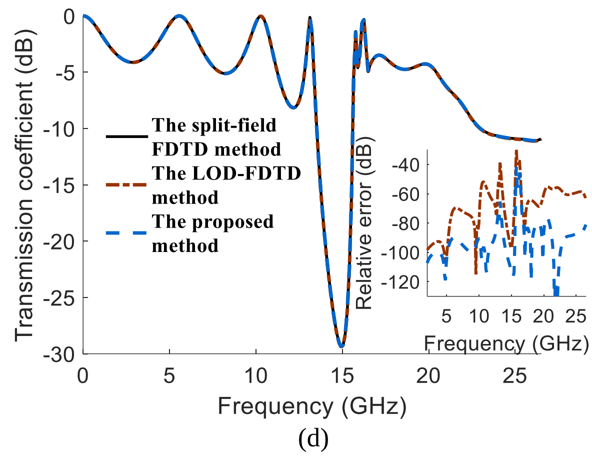


Fig. 2. Transmission coefficient and relative errors calculated by three methods: (a) θ=30°, (b) θ=45°, (c) θ=60°, and (d) θ=75°.

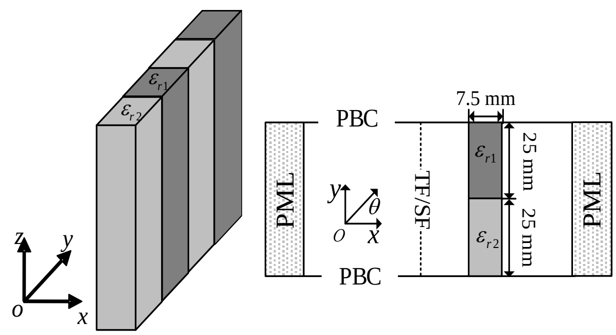


Fig. 3. Geometry of a dielectric frequency selective surfaces

Figure 4 shows the transmission coefficient and the relative error of the traditional SF FDTD method and the propose method with θ=45° and θ=75°. Table 2 provides the computational resources of the numerical simulation. It can be observed from Fig. 4 that the results of the proposed method are agreeable with the traditional SF FDTD method. Table 2 shows that the proposed method can greatly reduce runtime and memory storage compared with the traditional SF FDTD method because of the bigger time step size.

Table 2: CPU times and memory cost of the simulation of the second example

Method	Memory (kB)	CPU Time (s)	
		θ=45°	θ=75°
The traditional SF FDTD method	346	73.64	298.45
The proposed method	100	23.43	38.66

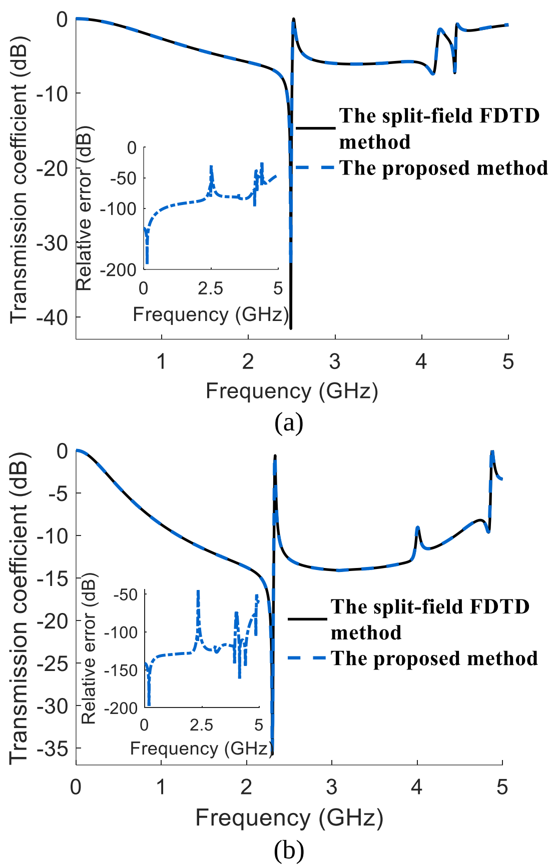


Fig. 4. Transmission coefficient and relative errors calculated by the traditional SF FDTD method and the proposed method: (a) θ=45° and (b) θ=75°.

V. CONCLUSIONS

In this paper, an efficient explicit leapfrog SF FDTD method for analyzing periodic structures' scattering problems is deduced. In comparisons with the traditional SF FDTD method and some unconditionally stable methods, the proposed method has better numerical performance and more concise implementation. Two examples verified the performance of this method in analyzing a PBG and a DFSS structure.

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