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A General ADE-FDTD with Crank-Nicolson Scheme for the Simulation of Dispersive Structures

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Abstract—A general auxiliary differential equation (ADE) finite difference time-domain (FDTD) method with Crank-Nicolson (CN) scheme is proposed to model electromagnetic wave propagation in dispersive materials in this paper. The proposed method introduces an ADE technique that establishes the relationship between the electric displacement vector and electric field intensity with a differential equation in dispersive media. The CN scheme applies only to Faraday's law, resulting in reduced memory usage and computing time. To validate the advantages of the proposed approach, two examples with plane wave propagation in dispersive media are calculated. Compared with the conventional ADE-CN-FDTD method, the results from our proposed method show its accuracy and efficiency for dispersive media simulation.

1. INTRODUCTION

The finite-difference time-domain (FDTD) method has been widely used in simulating and designing many electromagnetic devices [1]. However, the Courant-Friedrich-Levy stability condition restricts the time step making the CPU simulation prohibitively long. To eliminate this limitation, an unconditionally stable FDTD method with Crank-Nicolson scheme has been proposed [2–5]. This scheme has no limit on the time step size arising from stability considerations and has high numerical accuracy [5].

The CN scheme leads to a huge sparse matrix equation which is very challenging to solve. To solve the huge sparse matrix equation, a few efficient algorithms are used to implement the CN-FDTD method, such as Crank-Nicolson direct-splitting (CNDS) and Crank-Nicolson cycle-sweep-uniform (CNCSU) [3]. These algorithms use factorization-splitting leading to simple matrices at each sub-step. For method much simpler and more concise than original CN scheme, a new efficient algorithm for implementing 3-D Crank-Nicolson-based FDTD methods has been proposed [4]. In this method, auxiliary updating is introduced to reduce the flops count. The above methods are split- or sub-step. To improve the CPU efficiency and save memory, a new two-dimensional (2-D) unconditionally stable FDTD method based on CN scheme is proposed [5]. This method applies only to one of the Maxwell curl equations, and only one of the electric or magnetic fields needs to be updated during the iterations of the algorithm. Although this method improves the calculation efficiency, it cannot be used to model dispersive materials due to the lack of frequency-dependent relative dielectric constant. In [6], a novel ADE-FDTD with CN scheme is proposed for electromagnetic simulation of dispersive materials.

In this paper, by introducing auxiliary difference equation and applying the CN scheme to Faraday's law, a general auxiliary differential equation (ADE) finite-difference time-domain (FDTD) method with Crank-Nicolson (CN) scheme is proposed to model electromagnetic wave propagation in dispersive material. Compared to the conventional implementation, less CPU runtime is spent. The accuracy and efficiency of the proposed method are verified by simulating electromagnetic wave propagation in a variety of dispersive media.

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2. MATHEMATICAL FORMULATION

With lossless and dispersive media, the Maxwell's equations can be written as

$$j\omega\varepsilon_0\varepsilon_r(\omega)\mathbf{E}(\omega,\mathbf{r}) = \nabla\times\mathbf{H}(\omega,\mathbf{r}) \tag{1}$$

$$j\omega\mu_0\mathbf{H}(\omega,\mathbf{r}) = -\nabla\times\mathbf{E}(\omega,\mathbf{r}) \tag{2}$$

where ε_0 and μ_0 are the electric permittivity and magnetic permeability of free space, respectively. ε_r describes the relative dielectric constant and can be written in a general form as [7]

$$\varepsilon_r(\omega) = \varepsilon_\infty\left(1+\sum_{n}^{N_d}\frac{a_n}{b_n+j\omega c_n-d_n\omega^2}\right) \tag{3}$$

where ε_∞ is the infinite dielectric constant. a_n, b_n, c_n, and d_n are known constants. N_d is the number of poles. Substituting Eq. (3) into Eq. (1), we get

$$j\omega\varepsilon_0\varepsilon_\infty\mathbf{E}(\omega,\mathbf{r})+j\omega\varepsilon_0\varepsilon_\infty\sum_{n=1}^{N_d}\mathbf{S}_n(\omega,\mathbf{r}) = \nabla\times\mathbf{H}(\omega,\mathbf{r}) \tag{4}$$

where $\mathbf{S}$ is the auxiliary variable and can be written as

$$\mathbf{S}_n(\omega,\mathbf{r}) = \frac{a_n}{b_n+j\omega c_n-d_n\omega^2}\mathbf{E}(\omega,\mathbf{r}) \tag{5}$$

With the transition relationship from frequency domain to time domain ($j\omega\to\partial/\partial t$), Eqs. (2), (4), and (5) can be written as

$$\varepsilon_0\varepsilon_\infty\frac{\partial\mathbf{E}(t,\mathbf{r})}{\partial t}+\varepsilon_0\varepsilon_\infty\sum_{n=1}^{N_d}\frac{\partial\mathbf{S}_n(t,\mathbf{r})}{\partial t} = \nabla\times\mathbf{H}(t,\mathbf{r}) \tag{6}$$

$$\mu_0\frac{\partial\mathbf{H}(t,\mathbf{r})}{\partial t} = -\nabla\times\mathbf{E}(t,\mathbf{r}) \tag{7}$$

$$b_n\mathbf{S}(t,\mathbf{r})+c_n\frac{\partial\mathbf{S}(t,\mathbf{r})}{\partial t}+d_n\frac{\partial^2\mathbf{S}(t,\mathbf{r})}{\partial t^2} = a_n\mathbf{E}(t,\mathbf{r}) \tag{8}$$

For the sake of simplicity, in the following sections we will employ a 2-D TE$_z$ case and single pole dispersive media ($N_d = 1$) to describe the procedures for deriving the general ADE-CN-FDTD algorithm. By discretizing Eqs. (6)–(8) in time domain with some manipulations, we get

$$H_z^{n+0.5} = H_z^{n-0.5}+\frac{\Delta t}{\mu_0}\mathbf{D}^T\mathbf{E}^n \tag{9}$$

$$2\varepsilon_0\varepsilon_\infty(1+C_1)E_x^{n+1} = 2\varepsilon_0\varepsilon_\infty(1-C_1)E_x^n+2\varepsilon_0\varepsilon_\infty(1+C_2)S_x^n+2\varepsilon_0\varepsilon_\infty C_3S_x^{n-1}+2\Delta tD_yH_z^{n+0.5} \tag{10}$$

$$2\varepsilon_0\varepsilon_\infty(1+C_1)E_y^{n+1} = 2\varepsilon_0\varepsilon_\infty(1-C_1)E_y^n+2\varepsilon_0\varepsilon_\infty(1+C_2)S_y^n+2\varepsilon_0\varepsilon_\infty C_3S_y^{n-1}-2\Delta tD_xH_z^{n+0.5} \tag{11}$$

$$S_\xi^{n+1} = C_1E_\xi^{n+1}+C_1E_\xi^n-C_2S_\xi^n-C_3S_\xi^{n-1},\quad \xi=x,y \tag{12}$$

where $\mathbf{E}^n = [E_x^n, E_y^n]^T$, $C_1 = a_n\Delta t^2/(\Delta t^2b_n+2\Delta tc_n+2d_n)$, $C_2 = (\Delta t^2b_n-2\Delta tc_n-4d_n)/(\Delta t^2b_n+2\Delta tc_n+2d_n)$, $C_3 = 2d_n/(\Delta t^2b_n+2\Delta tc_n+2d_n)$. $\mathbf{D}^T = [D_y, -D_x]$, D_x and D_y are the first-order central finite-difference operators along x and y directions. Combining Eqs. (10) and (11) leads to

$$\mathbf{A}\mathbf{E}^{n+1} = \mathbf{B}\mathbf{E}^n+2\Delta t\mathbf{D}H_z^{n+0.5}+\mathbf{C}\mathbf{S}^n+\mathbf{F}\mathbf{S}^{n-1} \tag{13}$$

where $\mathbf{E}^{n+1} = [E_x^{n+1}, E_y^{n+1}]^T$, $\mathbf{S}^n = [S_x^n, S_y^n]^T$ and

$$\mathbf{A} = \begin{bmatrix}2\varepsilon_0\varepsilon_\infty(1+C_1) & 0\\ 0 & 2\varepsilon_0\varepsilon_\infty(1+C_1)\end{bmatrix},\quad \mathbf{B} = \begin{bmatrix}2\varepsilon_0\varepsilon_\infty(1-C_1) & 0\\ 0 & 2\varepsilon_0\varepsilon_\infty(1-C_1)\end{bmatrix},$$

$$\mathbf{C} = \begin{bmatrix}2\varepsilon_0\varepsilon_\infty(1+C_2) & 0\\ 0 & 2\varepsilon_0\varepsilon_\infty(1+C_2)\end{bmatrix},\quad \mathbf{F} = \begin{bmatrix}2\varepsilon_0\varepsilon_\infty C_3 & 0\\ 0 & 2\varepsilon_0\varepsilon_\infty C_3\end{bmatrix}.$$

By applying the CN scheme to Eq. (9), we have

$$H_z^{n+0.5} = H_z^{n-0.5} + \frac{\Delta t}{2\mu_0}\mathbf{D}^T\left(\mathbf{E}^{n+1} + \mathbf{E}^{n-1}\right) \tag{14}$$

Next, substitute Eq. (14) into Eq. (13) gives

$$\left(\mathbf{A} - \frac{\Delta t^2}{\mu_0}\mathbf{D}\mathbf{D}^T\right)\mathbf{E}^{n+1} = \mathbf{B}\mathbf{E}^n + 2\Delta t\mathbf{D}H_z^{n-0.5} + \frac{\Delta t^2}{\mu_0}\mathbf{D}\mathbf{D}^T\mathbf{E}^{n-1} + \mathbf{C}\mathbf{S}^n + \mathbf{F}\mathbf{S}^{n-1} \tag{15}$$

Enforcing Eq. (13) at time step $n-1/2$, i.e.,

$$2\Delta t\mathbf{D}H_z^{n-0.5} = \mathbf{A}\mathbf{E}^n - \mathbf{B}\mathbf{E}^{n-1} - \mathbf{C}\mathbf{S}^{n-1} - \mathbf{F}\mathbf{S}^{n-2} \tag{16}$$

And substitute Eq. (16) into Eq. (15), we have

$$\left(\mathbf{A} - \frac{\Delta t^2}{\mu_0}\mathbf{D}\mathbf{D}^T\right)\left(\mathbf{E}^{n+1} + \mathbf{E}^{n-1}\right) = \left(\mathbf{B} + \mathbf{A}\right)\mathbf{E}^n + \left(\mathbf{A} - \mathbf{B}\right)\mathbf{E}^{n-1} + \mathbf{C}\mathbf{S}^n + \left(\mathbf{F} - \mathbf{C}\right)\mathbf{S}^{n-1} - \mathbf{F}\mathbf{S}^{n-2} \tag{17}$$

By introducing an auxiliary field variable $\mathbf{e}$ as

$$\mathbf{e}^{n+1} = \mathbf{E}^{n+1} + \mathbf{E}^{n-1} \tag{18}$$

the updating equation reforms to:

$$\left(\mathbf{A} - \frac{\Delta t^2}{\mu_0}\mathbf{D}\mathbf{D}^T\right)\mathbf{e}^{n+1} = \left(\mathbf{B} + \mathbf{A}\right)\mathbf{E}^n + \left(\mathbf{A} - \mathbf{B}\right)\mathbf{E}^{n-1} + \mathbf{C}\mathbf{S}^n + \left(\mathbf{F} - \mathbf{C}\right)\mathbf{S}^{n-1} - \mathbf{F}\mathbf{S}^{n-2} \tag{19}$$

Split $-DD^T$ into two parts $-DD^T = \mathbf{M}_S + \mathbf{M}_M$, where

$$\mathbf{M}_S = \begin{bmatrix} -D_y^2 & 0 \\ 0 & -D_x^2 \end{bmatrix}, \quad \mathbf{M}_M = \begin{bmatrix} 0 & D_x D_y \\ D_x D_y & 0 \end{bmatrix} \tag{20}$$

Substituting Eq. (20) into Eq. (19) and utilizing the approximation $\mathbf{M}_M\mathbf{e}^{n+1} \approx 2\mathbf{M}_M\mathbf{E}^n$, we can obtain

$$\left(\mathbf{A} + \frac{\Delta t^2}{\mu_0}\mathbf{M}_s\right)\mathbf{e}^{n+1} = \left(\mathbf{B} + \mathbf{A} - \frac{2\Delta t^2}{\mu_0}\mathbf{M}_M\right)\mathbf{E}^n + \left(\mathbf{A} - \mathbf{B}\right)\mathbf{E}^{n-1} + \mathbf{C}\mathbf{S}^n + \left(\mathbf{F} - \mathbf{C}\right)\mathbf{S}^{n-1} - \mathbf{F}\mathbf{S}^{n-2} \tag{21}$$

With reference to Eq. [5], we can obtain the update equations of the proposed method as

$$\begin{aligned} &\left(2\varepsilon_0\varepsilon_\infty\left(1 + C_1\right) + \frac{2\Delta t^2}{\mu_0\Delta y^2}\right)e_x^{n+1}|_{i,j} - \frac{\Delta t^2}{\mu_0}\left(e_x^{n+1}|_{i,j+1} + e_x^{n+1}|_{i,j-1}\right) \\ =\ & 4\varepsilon_0\varepsilon_\infty E_x^n|_{i,j} - \frac{2\Delta t^2}{\Delta x\Delta y\mu_0}\left(E_y|_{i+1,j}^n - E_y|_{i,j}^n - E_y|_{i+1,j-1}^n + E_y|_{i,j-1}^n\right) + 4\varepsilon_0\varepsilon_\infty C_1 E_x^{n-1}|_{i,j} \\ &+ 2\varepsilon_0\varepsilon_\infty\left(1 + C_2\right)S_x^n|_{i,j} + 2\varepsilon_0\varepsilon_\infty\left(C_3 - 1 - C_2\right)S_x^{n-1}|_{i,j} - 2\varepsilon_0\varepsilon_\infty C_3 S_x^{n-2}|_{i,j} \end{aligned} \tag{22}$$

$$\begin{aligned} &\left(2\varepsilon_0\varepsilon_\infty\left(1 + C_1\right) + \frac{2\Delta t^2}{\mu_0\Delta y^2}\right)e_y^{n+1}|_{i,j} - \frac{\Delta t^2}{\mu_0}\left(e_y^{n+1}|_{i+1,j} + e_y^{n+1}|_{i-1,j}\right) \\ =\ & 4\varepsilon_0\varepsilon_\infty E_y^n|_{i,j} - \frac{2\Delta t^2}{\mu_0\Delta y\Delta x}\left(E_x|_{i,j+1}^n - E_x|_{i,j}^n - E_x|_{i-1,j+1}^n + E_x|_{i-1,j}^n\right) + 4\varepsilon_0\varepsilon_\infty C_1 E_y^{n-1}|_{i,j} \\ &+ 2\varepsilon_0\varepsilon_\infty\left(1 + C_2\right)S_y^n|_{i,j} + 2\varepsilon_0\varepsilon_\infty\left(C_3 - 1 - C_2\right)S_y^{n-1}|_{i,j} - 2\varepsilon_0\varepsilon_\infty C_3 S_y^{n-2}|_{i,j} \end{aligned} \tag{23}$$

where

$$E_\xi^{n+1}|_{i,j} = e_\xi^{n+1}|_{i,j} - E_\xi^{n-1}|_{i,j} \tag{24}$$

$$S_\xi^{n+1}|_{i,j} = C_1 E_\xi^{n+1}|_{i,j} + C_1 E_\xi^n|_{i,j} - C_2 S_\xi^n|_{i,j} - C_3 S_\xi^{n-1}|_{i,j} \tag{25}$$

Hence, the proposed method can be summarized into three steps. First, implicitly update x and y components of $\mathbf{e}$ using Eqs. (22) and (23). Second, explicitly update E_x and E_y with Eq. (24). Finally, the auxiliary variables are obtained from Eq. (25). Compared with the conventional ADE-CN-FDTD method in [8], the proposed method does not have the magnetic field, and only two tridiagonal matrix equations need to be solved. Compared with the novel ADE-CN-FDTD method in [6], the update equation of the proposed method includes E^{n-1} in Equations (22), (23) and E^{n+1} plus E^n instead of minus in Equation (25). Our proposed method is an alternative technique to simulate wave propagation in general dispersive media.

3. NUMERICAL RESULTS

In order to validate the effectiveness of the proposed method, we simulate the transient fields in a 2D cavity with dispersive media, as shown in Fig. 1. A sinusoidally modulated Gaussian pulse is used as an incident electric current profile

$$J_y(t) = \exp\left[-\left(\frac{t-T_c}{T_d}\right)^2\right]\sin 2\pi f_c(t-T_c) \tag{26}$$

where $T_d = 1/(2f_c)$, $T_c = 3T_d$ and $f_c = 10\,\text{GHz}$. The computational domain consists of 100×100 cells with a uniform cell size of $1.25 \times 1.25\,\text{cm}^2$. PEC boundary is utilized in both x and y directions. The problem is solved with both the conventional ADE-CN-FDTD and the proposed method. The dispersive material is described by the Lorentz model, in which the relative complex permittivity is given by

$$\varepsilon_r(\omega) = \varepsilon_\infty + (\varepsilon_s - \varepsilon_\infty)\frac{G_1\omega_1^2}{\omega_1^2 + 2j\delta_1\omega - \omega^2} \tag{27}$$

where $\varepsilon_s = 3$, $\varepsilon_\infty = 1.5$, $\omega_1 = 2 \times 10^9\,\text{rad/s}$, $G_1 = 0.4$ and $\delta_1 = 0.1\omega_1$.

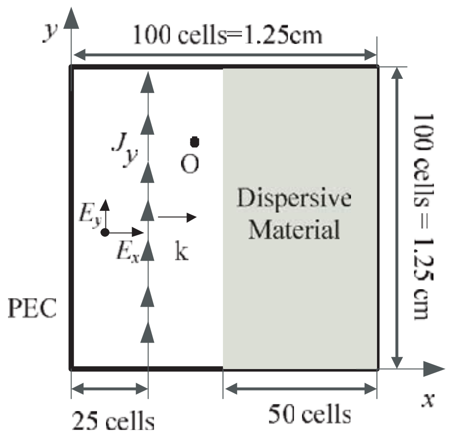

Figure 1. Diagram of computational domain for ADE-CN-FDTD.

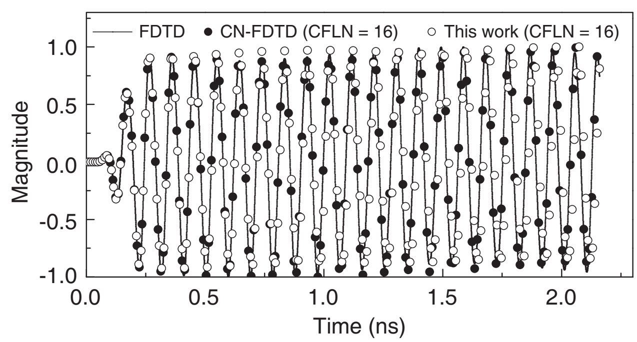

Figure 2. The transient fields calculated with conventional ADE-CN-FDTD and the proposed method for Lorentz model.

Figure 2 shows the calculated transient fields from both the conventional ADE-CN-FDTD and the proposed method at observation point O $(40\Delta x, 75\Delta y)$. Simulation results of the two methods agree well with each other. In order to reveal the computational accuracy of the proposed method, the calculated results for conventional ADE-FDTD method as benchmark are given in Fig. 2. Fig. 3 shows the relative difference of the transient field from the conventional ADE-CN-FDTD and proposed method. The relative difference of the transient field is defined as: $|\mathbf{E}_{\text{ADE-CN-FDTD}} - \mathbf{E}_{\text{ADE-FDTD}}|/\sum \mathbf{E}_{\text{ADE-FDTD}} \times 100\%$, where $\mathbf{E}_{\text{ADE-FDTD}}$ is the reference transient fields from ADE-FDTD, $\mathbf{E}_{\text{ADE-CN-FDTD}}$ the transient fields from the conventional ADE-CN-FDTD or the proposed method, and $\sum \mathbf{E}_{\text{ADE-FDTD}}$ the accumulation of the transient electric fields from ADE-FDTD.

Table 1 presents the required computational resource and computing time for numerical simulations. Compared with the conventional ADE-CN-FDTD in [8] with the Courant-Friedrich-Levy number (CFLN) of 8, for example, the proposed method with CFLN $= 8$ shows the reductions of 50% and 18% on computing time and memory usage, respectively. To investigate the accuracy of the proposed method, the resonant frequencies obtained through discrete Fourier transform for different methods are compared with each other, and the relative error of the resonant frequency is defined as $|f_{\text{ADE-CN-FDTD}} - f_{\text{ADE-FDTD}}|/f_{\text{ADE-FDTD}} \times 100\%$, where $f_{\text{ADE-FDTD}}$ is the reference frequency from ADE-FDTD, and $f_{\text{ADE-CN-FDTD}}$ is the resonant frequency from the conventional ADE-CN-FDTD [8] or the proposed method. It can be seen from Table 1 that the relative error becomes large when Δt increases in the conventional ADE-CN-FDTD or the proposed method.

Table 1. Comparison of the computational efforts for the 2-D cavity loaded Lorentz material.

Method	Δt (ps)	Marching steps	Memory (MB)	Computing time (s)	Error (%)
FDTD	0.2	10800	1.6	29	–
CN-FDTD (CFLN = 8)	1.6	1350	3.8	40	0.09
CN-FDTD (CFLN = 16)	3.2	675	3.8	31	0.38
This work (CFLN = 8)	1.6	1350	3.1	20	0.23
This work (CFLN = 16)	3.2	675	3.1	10	0.94

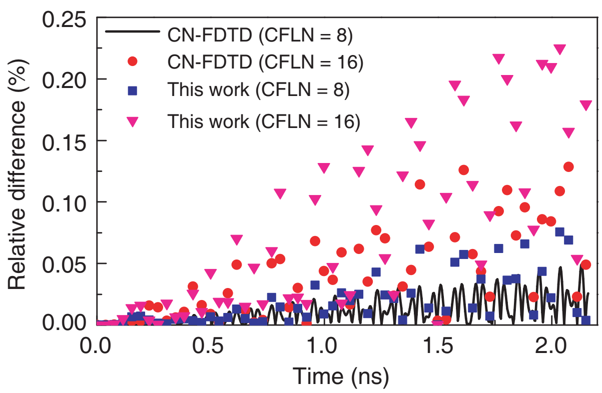

Figure 3. The relative difference calculated with conventional ADE-CN-FDTD and the proposed method for Lorentz model.

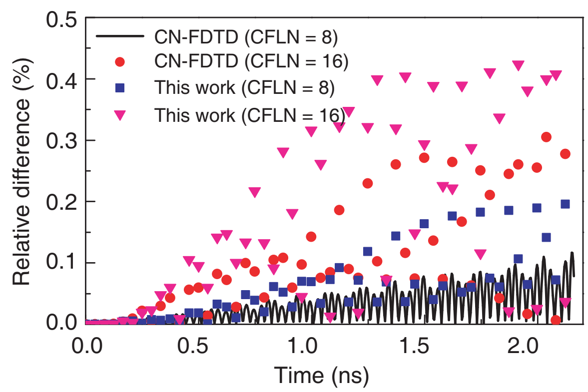

Figure 4. The relative difference calculated with conventional ADE-CN-FDTD and the proposed method for Debye model.

As the second example, we employ a Debye model replacing Lorentz material in the first example. The relative complex permittivity of Debye model is given as

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + j\omega\tau} \tag{28}$$

where $\varepsilon_s = 4.301$, $\varepsilon_\infty = 4.096$, and $\tau = 2.294 \times 10^{-9}$. Fig. 4 shows the relative difference of transient fields from both the conventional ADE-CN-FDTD and the proposed method. From their profiles, one can find that the accuracy of the proposed method is verified. Table 2 presents the required computational resource and computing time for the numerical simulations. The proposed method shows much improvement in computation efficiency compared to the ADE-CN-FDTD. All calculations were performed on intel (R) Core (TM) i5-4210 CPU with 8 GB RAM.

Table 2. Comparison of the computational efforts for the 2-D cavity loaded Debye material.

Method	Δt (ps)	Marching steps	Memory (MB)	Computing time (s)	Error (%)
FDTD	0.2	10800	1.6	29	–
CN-FDTD ((CFLN = 8)	1.6	1350	3.8	46	0.09
CN-FDTD (CFLN = 16)	3.2	675	3.8	31	0.19
This work (CFLN = 8)	1.6	1350	3.1	20	0.16
This work (CFLN = 16)	3.2	675	3.1	10	0.22

4. CONCLUSION

A general ADE-FDTD method based on the CN scheme for dispersive media is presented in this paper. Compared with the conventional ADE-CN-FDTD, the proposed method greatly increases computing efficiency without degrading the calculation accuracy. Two numerical examples have been presented to verify the accuracy and efficiency of the proposed method.

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