Implicit high-order unconditionally stable complex envelope algorithm for solving the time-dependent Maxwell's equations

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Received August 26, 2008; revised October 17, 2008; accepted October 18, 2008; posted October 22, 2008 (Doc. ID 100616); published November 19, 2008

Based on the Padé approximation and multistep method, we propose an implicit high-order unconditionally stable complex envelope algorithm to solve the time-dependent Maxwell's equations. Unconditional numerical stability can be achieved simultaneously with a high-order accuracy in time. As we adopt the complex envelope Maxwell's equations, numerical dispersion and dissipation are very small even at comparatively large time steps. To verify the capability of our algorithm, we compare the results of the proposed method with the exact solutions. © 2008 Optical Society of America

OCIS codes: 000.4430, 230.1480, 240.6700.

The well-known class of algorithms to solve time-dependent Maxwell's equations (TDMEs) is based on the finite-difference time-domain (FDTD) method proposed by Yee [1]. The FDTD method is a simple, robust, and powerful technique to simulate transient electromagnetic (EM) phenomena [2]. However, since the FDTD method is an explicit time-stepping technique, its time step is limited by the Courant–Friedrichs–Lewy (CFL) stability condition [2]. As a result, the FDTD may require a large number of iterations in time, especially when fine geometries are involved. To remove the CFL stability condition, several time-domain techniques have been developed. Kole *et al.* and De Raedt *et al.* [3–5] presented a family of unconditionally stable algorithms that solve the TDME through the application of orthogonal transformations. Although this method can produce a high-order approximation, the time-evolution operator is not always an orthogonal transformation. Moreover, this method needs to solve many exponential matrices to obtain a high-order approximation.

In this Letter, we propose an implicit high-order unconditionally stable complex envelope algorithm to solve the TDME based on the Padé approximation and multistep method. Unconditional numerical stability can be achieved simultaneously with a high-order accuracy in time. As we adopt the complex envelope Maxwell's equations, numerical dispersion and dissipation are very small even at large time steps. Thus, the upper bound of the time step is implied only by the required numerical accuracy. Meanwhile, we compared the results of our algorithm with exact solutions, which agree well with each other.

Maxwell's curl equations for the envelopes of the EM fields **E** and **H** in linear, isotropic, lossless, and nondispersive media are given in the differential form by

$$\frac{\partial \mathbf{H}}{\partial t} + j\omega \mathbf{H} = -\frac{1}{\mu}\nabla \times \mathbf{E}, \tag{1}$$

$$\frac{\partial \mathbf{E}}{\partial t} + j\omega \mathbf{E} = \frac{1}{\epsilon}\nabla \times \mathbf{H}, \tag{2}$$

where ϵ and μ are the permittivity and permeability and ω denotes the carrier frequency. The complex envelope TDME can be rewritten as

$$\frac{\partial}{\partial t}\begin{pmatrix}\mathbf{H}(t)\\ \mathbf{E}(t)\end{pmatrix} = \begin{pmatrix} -j\omega & -\frac{1}{\mu}\nabla \times \\ \frac{1}{\epsilon}\nabla \times & -j\omega \end{pmatrix}\begin{pmatrix}\mathbf{H}(t)\\ \mathbf{E}(t)\end{pmatrix} \equiv M\begin{pmatrix}\mathbf{H}(t)\\ \mathbf{E}(t)\end{pmatrix}, \tag{3}$$

and using $\Psi(t)=[\mathbf{H}(t),\mathbf{E}(t)]^T$, Eq. (3) becomes

$$\frac{\partial}{\partial t}\Psi(t) = M\Psi(t). \tag{4}$$

The formal solution of Eq. (4) is given by

$$\Psi(t+\tau) = \exp(\tau M)\Psi(t). \tag{5}$$

In a numerical procedure, the time-evolution operator $\exp(\tau M)$ can be solved by Padé approximation [6]

$$\exp_{1/1}(\tau M) = \frac{I + \frac{1}{2}\tau M}{I - \frac{1}{2}\tau M}, \tag{6}$$

$$\exp_{2/2}(\tau M) = \frac{\left[I - \frac{-3+\sqrt{3}i}{12}\tau M\right]\left[I - \frac{-3-\sqrt{3}i}{12}\tau M\right]}{\left[I + \frac{-3+\sqrt{3}i}{12}\tau M\right]\left[I + \frac{-3-\sqrt{3}i}{12}\tau M\right]}, \tag{7}$$

0146-9592/08/232755-3/$15.00

$$\exp_{n/n}(\tau M) = \frac{(I - a_n \tau M)\cdots(I - a_2 \tau M)(I - a_1 \tau M)}{(I + a_n \tau M)\cdots(I + a_2 \tau M)(I + a_1 \tau M)}, \quad (8)$$

where I denotes the unit matrix. If we execute Eq. (6) as an approximation, the implicit scheme of Eq. (5) can be reduced to the Crank–Nicolson method [2], which is unconditionally stable and second order in time. Equation (8) has the $2n$th-order accuracy in time, and the coefficients a_n are the reciprocal of the factor decomposition coefficients for the numerator of the Padé operator.

Thus, the unknown field $\Psi(t+\tau)$ is related to the known field $\Psi(t)$ as follows:

$$\Psi(t + \tau) = \frac{(I - a_n \tau M)\cdots(I - a_2 \tau M)(I - a_1 \tau M)}{(I + a_n \tau M)\cdots(I + a_2 \tau M)(I + a_1 \tau M)}\Psi(t). \quad (9)$$

The $2n$th-order Padé propagator may be decomposed into an n-step algorithm by the multistep method for which the ith partial step takes the form [7]

$$\Psi\left(t + \frac{i}{n}\tau\right) = \frac{(I - a_i \tau M)}{(I + a_i \tau M)}\Psi\left(t + \frac{i-1}{n}\tau\right). \quad (10)$$

Each such partial step is unitary and tridiagonal. These two important properties imply that the resulting algorithm is unconditionally stable and Eq. (10) can be solved efficiently by the Thomas algorithm [8].

In this section, we present the details of the implementation of our algorithm. To demonstrate the basic idea of our algorithm, we consider a one-dimensional (1D) system along the x direction. In this case, the complex envelope TDME for TM mode are reduced to two independent sets of first-order differential equations. Using the second-order central-difference approximation to the first derivative with respect to x, we obtain

$$\frac{\partial H_y(i,t)}{\partial t} = \frac{1}{\mu_i}\left[\frac{1}{\Delta x}(E_z(i+1,t) - E_z(i-1,t))\right] - j\omega H_y(i,t), \quad (11)$$

$$\frac{\partial E_z(j,t)}{\partial t} = \frac{1}{\epsilon_j}\left[\frac{1}{\Delta x}(H_y(j+1,t) - H_y(j-1,t))\right] - j\omega E_z(j,t), \quad (12)$$

where the integers i and j label the grid points and Δx denotes the distance between two next-nearest neighbor lattice points. The electric field vanishes at the boundaries, which is required by the boundary conditions. Equations (11) and (12) can be combined into one equation in the form of Eq. (5) by introducing the n-dimensional vector

$$\Psi(i,t) = \begin{cases} H_y(i,t) & i \text{ odd} \\ E_z(i,t) & i \text{ even} \end{cases}. \quad (13)$$

The ith element of $\Psi(i,t)$ is given by the inner product $\Psi(i,t) = e_i^T \cdot (t)$, where e_i denotes the ith unit vector in the n-dimensional vector space. Using this notation, the matrix M is given by

$$M = \sum_{i=1}^{n-1} [\alpha_i e_i e_{i+1}^T - \alpha_{i+1} e_{i+1} e_i^T + \beta e_i e_i^T], \quad (14)$$

where

$$\alpha_i = (1/\Delta x)(1/\eta_i), \quad \beta = -j\omega, \quad \text{and} \quad \eta_i = \begin{cases} \mu_i & i \text{ odd} \\ \epsilon_i & i \text{ even} \end{cases}.$$

In a two-dimensional (2D) TDME, the matrix of M is divided into two matrices M_x and M_y. Therefore, Eq. (5) reads

$$\Psi(t + \tau) = \exp(\tau M_x + \tau M_y)\Psi(t). \quad (15)$$

With an application of the locally one-dimensional scheme (LOD), Eq. (15) can be solved in two steps. In each half step of the LOD, we move forward only in the x or y direction. Therefore, we can repeat the 1D scheme to update the time step.

In the following, we present several simulated results to test our algorithm. As the TDME are scale invariant, the length and the velocity of light in vacuum are in units of λ and c, respectively. Time is given in units of $t_0 = \lambda/c$. To examine the stability and the numerical error of our scheme, we let an incident Gaussian pulse propagate in vacuum. Figure 1 shows the exact and the numerical solutions of electric amplitude when the wave propagates 200 time units. The results demonstrate that our scheme will remain stable for long time propagation even at large time steps. Table 1 gives the error $L_2 = \sqrt{(1/N)\Sigma_{i=1}^{N}(E_i^{\text{exact}} - E_i^{\text{num}})^2}$ for four different time steps, where E_i^{exact} and E_i^{num} are the exact and the numerical solutions. The mesh grid is chosen very small so that the error from spatial integration can be neglected. In all three cases a fourth-order in the time convergence rate of the proposed algorithm is observed as demonstrated by the data in the third column of Table 1.

Figure 2 shows the numerical dispersion and dissipation errors in different orders of time. We compare results using Kole *et al.*'s method [3] with results obtained by our algorithm. Although the time step of Kole *et al.*'s method is far smaller than that of our al-

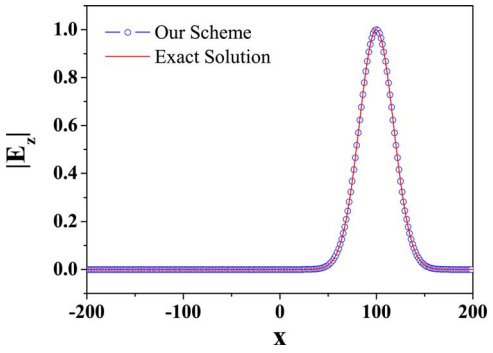

Fig. 1. (Color online) Exact and numerical solutions of electric amplitude when the wave propagates 200 time units in vacuum, where the mesh size and time step are $\Delta x = 0.0025$ and $\Delta t = 8$, respectively.

Table 1. Time Step Refinement Analysis for a 1D System

Time Step (Δt)	L_2 Error	Order
8	6.4645E−7	—
4	4.2725E−8	3.9194
2	2.9087E−9	3.8766
1	1.9863E−10	3.8722

gorithm, the dispersion and dissipation errors are much larger than those of our algorithm. The real time steps in second-order accuracy for both Kole *et al.*'s method and our scheme are one quarter of the time steps in Fig. 2. That is the reason why the second-order dissipation curve appears to be lower than the fourth-order dissipation curve in Fig. 2(a).

For the fourth-order in time scheme, both dispersion and dissipation errors are very small at comparatively large time steps. If we increase the spatial resolution, which is demanded in problems with detailed geometries, the numerical dispersion error can decrease further. Standard FDTD methods have no dissipation because it applies Yee leapfrog time stepping [2], but the time step is limited by the CFL stability condition. In contrast, dissipation occurs in our scheme because of the Padé approximation, but it remains very small even for large time steps.

Scattering and/or transmission of EM fields in the presence of an object are one of the main applications of the FDTD method [2]. The inset of Fig. 3 shows a quarter-wave reflector that consists of alternating layers of two materials with refractive indices of $\sqrt{2}$ and 1.0. Figure 3 compares the transmission of the quarter-wave reflector calculated by the transfer-matrix method (TMM) and by our scheme. The time step and mesh size for our scheme are 8 and 0.01, respectively. Clearly, the result of our scheme is consistent with that of the TMM calculations.

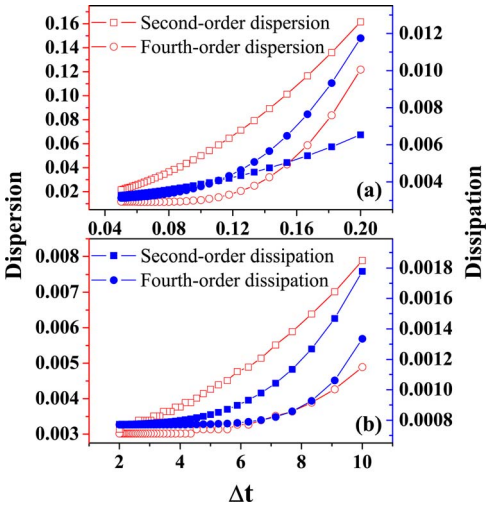

Fig. 2. (Color online) Numerical dispersion and dissipation error in different orders in time, where mesh size and pulse width are $\Delta x = 0.0025$ and $t_p = 25$, respectively. (a) Kole *et al.*'s method [3], (b) our scheme.

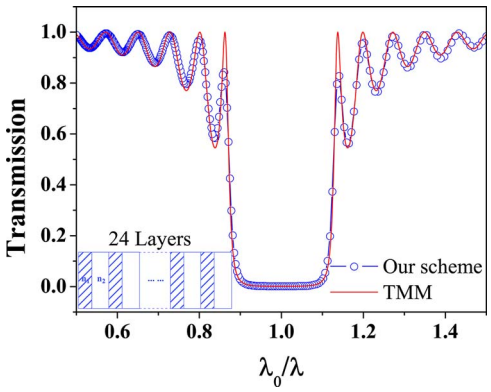

Fig. 3. (Color online) Transmission curves of the quarter-wave reflector obtained by TMM and our scheme, where the mesh size and time step for our scheme are $\Delta x = 0.01$ and $\Delta t = 8$, respectively. Inset, quarter-wave reflector.

In conclusion, we presented a novel algorithm to solve the TDME based on the Padé approximation and multistep method. Unconditional numerical stability can be achieved simultaneously with high-order accuracy in time. As we adopt the complex envelope Maxwell's equations, the mesh size can be chosen very small to account for detailed geometries in the actual numerical computation. Most importantly, in contrast to many conventional methods, the time step can be set very large to improve the computational efficiency. Even for large time steps the numerical dispersion and dissipation remain very small. Using higher-order schemes, the time step could be increased even further.

This research was supported by the National Natural Science Foundation of China (NNSFC) (grant 60678025), Chinese National Key Basic Research Special Fund (grant 2006CB921703), Program for New Century Excellent Talents in University, Arizona Technology and Research Initiative Fund, and the United States Air Force Office of Scientific Research (USAFOSR) (grants FA9550-07-1-0010 and FA9550-04-1-0213).

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