Numerical Dispersion Analysis for the 3-D High-Order WLP-FDTD Method

Wei-Jun Chen^{1, *}, Jun Quan², and Shi-Yu Long¹

Abstract—In this paper, a theoretical analysis of numerical dispersion of the three-dimensional (3-D) high-order finite-difference time-domain (FDTD) method with weighted Laguerre polynomials (WLPs) is presented. The phase velocity of numerical wave modes is relevant to the direction of wave propagation, grid discretization and time-scale factor. The formula to determine a suitable time-scale factor is derived. By a theoretical evaluation, the dispersion errors for the 3-D high-order WLP-FDTD scheme with different time-scale factors are obtained. Finally, one numerical example is included to validate the effectiveness of the theoretical solution of the time-scale factor.

1. INTRODUCTION

The finite-difference time-domain (FDTD) method has been widely used for electromagnetic modeling in the last two decades [1]. However, because of Courant-Friedrich-Levy (CFL) stability constraint, the conventional FDTD is not very suitable for electromagnetic problems which involve fine grid division. To eliminate the limitation, an unconditionally stable FDTD method using weighted Laguerre polynomials (WLPs) has been proposed [2]. This method does not deal with time steps and is more efficient than the conventional FDTD method when analyzing multiscale structures.

WLP-FDTD leads to a large sparse matrix equation, which is expensive to solve. To overcome this problem, the factorization-splitting technique [3, 4] and domain decomposition scheme [5] are implemented in WLP-FDTD. They turn the large sparse matrix into several small ones while keeping the same number of unknowns. To reduce the number of unknowns, WLP-FDTDs combined with scaling functions [6] and mixed-order scheme [7] are introduced. With the reduction of the sampling density in space domain, the produced sparse matrix with a smaller size can result in an efficient solution.

For the high-order WLP-FDTD method with fourth-order central difference in space domain [7], a numerical dispersion analysis for the 3-D case is presented in this paper. Different from the numerical dispersion in FDTD only involving the direction of wave propagation and grid discretization, the time-scale factor s plays an important role in high-order WLP-FDTD and it affects dispersion errors to a great extent. Resonant frequencies in an air-filled cubic cavity are calculated to show the importance of correctly choosing the time-scale factor s.

2. NUMERICAL DISPERSION ANALYSIS

For simplicity, assume a linear, isotropic, nondispersive, and lossless medium, the 3-D Maxwell's equations in Laguerre-domain can be written as [8]

$$E_x^p|_{x,y,z} = \frac{2}{s\varepsilon} \left[\frac{\partial H_z^p|_{x,y,z}}{\partial y} - \frac{\partial H_y^p|_{x,y,z}}{\partial z} \right] - 2 \sum_{k=0, p>0}^{p-1} E_x^k|_{x,y,z}$$
(1a)

Received 20 September 2015, Accepted 21 October 2015, Scheduled 22 October 2015

^{*} Corresponding author: Wei-Jun Chen (chenw_j@163.com).

¹ School of Information Science and Technology, Lingnan Normal University, Zhanjiang 524048, China. ² School of Physics Science and Technology, Lingnan Normal University, Zhanjiang 524048, China.

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$$E_y^p |_{x,y,z} = \frac{2}{s\varepsilon} \left[\frac{\partial H_x^p |_{x,y,z}}{\partial z} - \frac{\partial H_z^p |_{x,y,z}}{\partial x} \right] - 2 \sum_{k=0, p>0}^{p-1} E_y^k |_{x,y,z}$$
(1b)

$$E_z^p|_{x,y,z} = \frac{2}{s\varepsilon} \left[\frac{\partial H_y^p|_{x,y,z}}{\partial x} - \frac{\partial H_x^p|_{x,y,z}}{\partial y} \right] - 2 \sum_{k=0,\,p>0}^{p-1} E_z^k|_{x,y,z}$$
(1c)

$$H_x^p|_{x,y,z} = \frac{2}{s\mu} \left[\frac{\partial E_y^p|_{x,y,z}}{\partial z} - \frac{\partial E_z^p|_{x,y,z}}{\partial y} \right] - 2 \sum_{k=0,\,p>0}^{p-1} H_x^k|_{x,y,z} \tag{1d}$$

$$H_y^p|_{x,y,z} = \frac{2}{s\mu} \left[\frac{\partial E_z^p|_{x,y,z}}{\partial x} - \frac{\partial E_x^p|_{x,y,z}}{\partial z} \right] - 2 \sum_{k=0, p>0}^{p-1} H_y^k|_{x,y,z}$$
(1e)

$$H_z^p|_{x,y,z} = \frac{2}{s\mu} \left[\frac{\partial E_x^p|_{x,y,z}}{\partial y} - \frac{\partial E_y^p|_{x,y,z}}{\partial x} \right] - 2 \sum_{k=0,p>0}^{p-1} H_z^k|_{x,y,z}$$
(1f)

where ε and μ are the electric permittivity and magnetic permeability, respectively. s is the time-scale factor and p is the order of Laguerre functions. Considering the monochromatic wave, we expand E_x^p , E_y^p , E_z^p , H_x^p , H_y^p and H_z^p into a discrete set of Fourier modes as follows [9, 10]:

$$\left\{E_x^p, E_y^p, E_z^p, H_x^p, H_y^p, H_z^p \mid_{m,n,l}\right\} = \left\{e_x^p, e_y^p, e_z^p, h_x^p, h_y^p, h_z^p\right\} e^{j_0(mk\Delta x\sin\theta\cos\varphi + nk\Delta y\sin\theta\sin\varphi + lk\Delta z\cos\theta)}$$
(2)

where (m, n, l) denotes the spatial index of a field component; Δx , Δy , and Δz are the spatial meshing sizes along the x- and y-, and z-axes; $j_0 = \sqrt{-1}$, k is the wavenumber; θ is the angle between the propagation direction and z-axis; φ is the angle between the propagation direction and xz plane. Inserting (2) into (1) with the fourth-order central-difference discretization [11, 12], we get

$$e_x^p - j_0 \frac{A_y}{6s\varepsilon\Delta y} h_z^p + j_0 \frac{A_z}{6s\varepsilon\Delta z} h_y^p = -2 \sum_{k=0, p>0}^{p-1} e_x^k$$
(3a)

$$e_y^p - j_0 \frac{A_z}{6s\varepsilon\Delta z} h_x^p + j_0 \frac{A_x}{6s\varepsilon\Delta x} h_z^p = -2\sum_{k=0, p>0}^{p-1} e_y^k$$
(3b)

$$e_z^p - j_0 \frac{A_x}{6s\varepsilon\Delta x} h_y^p + j_0 \frac{A_y}{6s\varepsilon\Delta y} h_x^p = -2 \sum_{k=0, p>0}^{p-1} e_z^k$$
(3c)

$$h_x^p - j_0 \frac{A_z}{6s\mu\Delta z} e_y^p + j_0 \frac{A_y}{6s\mu\Delta y} e_z^p = -2 \sum_{k=0, p>0}^{p-1} h_x^k$$
(3d)

$$h_y^p - j_0 \frac{A_x}{6s\mu\Delta x} e_z^p + j_0 \frac{A_z}{6s\mu\Delta z} e_x^p = -2 \sum_{k=0, p>0}^{p-1} h_y^k$$
(3e)

$$h_{z}^{p} - j_{0} \frac{A_{y}}{6s\mu\Delta y} e_{x}^{p} + j_{0} \frac{A_{x}}{6s\mu\Delta x} e_{y}^{p} = -2 \sum_{k=0, p>0}^{p-1} h_{z}^{p}$$
(3f)

where $A_{\xi} = 27 \sin(0.5k_{\xi}\Delta\xi) - \sin(1.5k_{\xi}\Delta\xi), \ \xi = x, y, z$. Equations (3) can be written in a matrix form as

$$\mathbf{A}\mathbf{X}^p = \sum_{k=0,\,p>0}^{p-1} \mathbf{X}^k \tag{4}$$

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where
$$\mathbf{X}^{p} = [e_{x}^{p}, e_{y}^{p}, e_{z}^{p}, h_{y}^{p}, h_{y}^{p}]^{T}, \mathbf{X}^{k} = [e_{x}^{k}, e_{y}^{k}, e_{z}^{k}, h_{x}^{k}, h_{y}^{k}, h_{z}^{k}]^{T}$$
 and

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 0 & 0 & a_{15} & -a_{34} \\ 0 & 1 & 0 & -a_{15} & 0 & a_{26} \\ 0 & 0 & 1 & a_{34} & -a_{26} & 0 \\ a_{51} & 0 & -a_{62} & 0 & 1 & 0 \\ -a_{43} & a_{62} & 0 & 0 & 0 & 1 \end{bmatrix}$$
. Here, $a_{15} = j_{0}A_{z}/(6s\epsilon\Delta z), \ a_{34} = j_{0}A_{y}/(6s\epsilon\Delta y),$
 $a_{26} = j_{0}A_{x}/(6s\epsilon\Delta x), \ a_{51} = j_{0}A_{z}/(6s\mu\Delta z), \ a_{43} = j_{0}A_{y}/(6s\mu\Delta y) \text{ and } a_{62} = j_{0}A_{x}/(6s\mu\Delta x).$
While $p = 0, 1, \dots, N - 1, N$, where N is the largest order of Laguerre functions, we have

$$\begin{bmatrix} \mathbf{A} & 0 & 0 & \dots & 0 & 0 & 0 \\ -\mathbf{I} & \mathbf{A} & 0 & \dots & 0 & 0 & 0 \\ -\mathbf{I} & -\mathbf{I} & \mathbf{A} & \dots & 0 & 0 & 0 \\ -\mathbf{I} & -\mathbf{I} & \mathbf{A} & \dots & 0 & 0 & 0 \\ -\mathbf{I} & -\mathbf{I} & -\mathbf{I} & -\mathbf{I} & -\mathbf{I} & \mathbf{A} & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ -\mathbf{I} & -\mathbf{I} & -\mathbf{I} & -\mathbf{I} & -\mathbf{I} & \mathbf{A} & 0 \end{bmatrix} \begin{bmatrix} \mathbf{X}^{0} \\ \mathbf{X}^{1} \\ \mathbf{X}^{2} \\ \vdots \\ \mathbf{X}^{N-1} \\ \mathbf{X}^{N} \end{bmatrix} = 0$$
(5)

where **I** is a 6×6 identity matrix. For a nontrivial solution of homogeneous Equation (5), the determinant of its coefficient matrix should be zero, thus leading to $|\mathbf{A}|^{N+1} = 0$. Consequently, it can be derived

$$\frac{729\sin^2(0.5k_x\Delta x)}{\Delta x^2} + \frac{\sin^2(1.5k_x\Delta x)}{\Delta x^2} - \frac{54\sin(0.5k_x\Delta x)\sin(1.5k_x\Delta x)}{\Delta x^2} + \frac{729\sin^2(0.5k_y\Delta y)}{\Delta y^2} + \frac{\sin^2(1.5k_y\Delta y)}{\Delta y^2} - \frac{54\sin(0.5k_y\Delta y)\sin(1.5k_y\Delta y)}{\Delta y^2} + \frac{729\sin^2(0.5k_z\Delta z)}{\Delta z^2} + \frac{\sin^2(1.5k_z\Delta z)}{\Delta z^2} - \frac{54\sin(0.5k_z\Delta z)\sin(1.5k_z\Delta z)}{\Delta z^2} = -36s^2\varepsilon\mu$$

$$(6)$$

While $\Delta x = \Delta y = \Delta z \rightarrow 0$ in (6), we get the theoretical solution of the time-scale factor

$$s_0 = |\mathrm{Im}(s)| = \frac{2k}{\sqrt{\varepsilon_0 \mu_0}} = 4\pi f_0$$
 (7)

where f_0 is the operating frequency. It can be noticed in (6) that the numerical dispersion of high-order WLP-FDTD is related to the propagation direction, sampling density in space domain and time-scale factor. The relative error of the numerical phase velocity can be written as

$$\delta_{r} = \left| \frac{v_{p} - c}{c} \right| = \left| \frac{s_{0}}{24\pi s\delta} \sqrt{ \begin{bmatrix} 729 \sin^{2}(\pi\delta\sin\theta\cos\varphi) + \sin^{2}(3\pi\delta\sin\theta\cos\varphi) \\ -54\sin(\pi\delta\sin\theta\cos\varphi) \sin(3\pi\delta\sin\theta\cos\varphi) \\ +729 \sin^{2}(\pi\delta\sin\theta\sin\varphi) + \sin^{2}(3\pi\delta\sin\theta\sin\varphi) \\ -54\sin(\pi\delta\sin\theta\sin\varphi) \sin(3\pi\delta\sin\theta\sin\varphi) \\ +729 \sin^{2}(\pi\delta\cos\theta) + \sin^{2}(3\pi\delta\cos\theta) \\ -54\sin(\pi\delta\cos\theta) \sin(3\pi\delta\cos\theta) \end{bmatrix} \right| - 1$$
(8)

where v_p is the numerical phase velocity, c is the speed of light in free space, $\delta = \Delta x / \lambda_0 = \Delta y / \lambda_0 = \Delta z / \lambda_0$ and λ_0 is the operating wavelength.

Figure 1 shows the relative errors of the numerical phase velocity of the 3-D high-order WLP-FDTD method with different s. Compared to low-order WLP-FDTD [9], few grid cells per wavelength are required in the high-order scheme to obtain acceptable accuracy. From Fig. 1, it is seen that the time-scale factor s affects dispersion errors to a great extent.

3. NUMERICAL RESULTS

To validate the importance of correctly choosing the time-scale factor s in the high-order scheme, resonance frequencies of a 3-D air filled cubic cavity with sides equal to 8 cm are calculated. A sinusoidally modulated Gaussian pulse is used as an incident electric current profile:

$$J_x(t) = e^{-\left(\frac{t-T_c}{T_d}\right)^2} \sin\left[2\pi f_c(t-T_c)\right]$$
(9)



Figure 1. Relative error of the numerical phase velocity of high-order WLP-FDTD versus φ and θ with different s. Top panel: $\delta = 1/6$; Middle panel: $\delta = 1/7$; Bottom panel: $\delta = 1/8$.

	TE_{101}		TE_{111}	
	Solution (MHz)	Error $(\%)$	Solution (MHz)	Error $(\%)$
Analytic	2.6504		249.89	
$0.98s_0$	2.6562	0.22	248.98	1.36
$0.99s_{0}$	2.6552	0.18	248.98	1.28
s_0	2.6548	0.17	249.13	1.23
$1.01s_0$	2.6562	0.22	249.05	1.31
$1.02s_0$	2.6565	0.23	249.03	1.32

Table 1. Comparison between different time-scale factors.

where $T_d = 1/(2f_c)$, $T_c = 3T_d$ and $f_c = 3$ GHz. We choose the time duration $T_f = 6$ ns (T_f is defined in [2]). Assuming the maximum operating frequency $f_{\text{max}} = 9$ GHz, we can obtain $s_0 = 1.131 \times 10^{11}$ with (7) and N = 178 from [9]. In this example, uniform cubic cells with $\Delta x = \Delta y = \Delta z = 1$ cm are used to divide the 3-D space domain.

For high-order WLP-FDTD with different time-scale factor s, Table 1 shows the calculated resonance frequencies and relative errors. In Table 1, the relative errors are the smallest ones while the time-scale factor s is chosen as the theoretical solution s_0 .

4. CONCLUSION

In this paper, with the fourth-order central difference in space domain, the numerical dispersion of 3-D high-order WLP-FDTD is analyzed, and the relationship between the time-scale factor and operating frequency is obtained. The suitable selection of the time-scale factor leads to low numerical dispersion errors. Moreover, if there exist material interfaces and boundaries in space domain, their handling in high-order scheme should also be involved to measure the algorithm performance [13].

ACKNOWLEDGMENT

The work is supported by the NSF of China (Grant No. 11304276) and the GDNSF of China (Grant No. 2014A030307035), the Cultivation of Innovative Talents in Colleges and Universities of Guangdong (Grant No. LYM10098) and the Science Foundation of Lingman Normal University, China (Grant No. ZL1104).

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