Truncation Error Analysis of a Pre-Asymptotic Higher-Order Finite Difference Scheme for Maxwell's Equations

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Abstract ─ Pre-asymptotic higher-order methods are useful to the mitigation of numerical dispersion error in large-scale Finite-Difference Time-Domain (FDTD) simulations. Its truncation error is shown in this study to be $\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta s^2)$ in general. In the limiting case where the Courant-Friedrichs-Levy number approaches to zero, it becomes $\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta s^4)$.

Index Terms ─ FDTD, higher-order, pre-asymptotic, truncation error.

I. INTRODUCTION

Numerical dispersion error is a major concern in large-scale finite-difference simulations of wave propagation and scattering problems [1]. For its mitigation, various techniques based on higher-order finite-difference schemes and non-canonical grids have been proposed in past decades [2]-[6]. However, the inherent frequency dependency and angle dependency (anisotropy) of their dispersion properties may not be desired in practical applications, such as those involving high-permittivity biological bodies at high frequency. For instance, their dispersion errors decrease at lower frequency, where the electrical size of certain geometry is smaller and the significance of dispersion error diminishes. It is preferred to have less dispersion error at higher frequency rather than lower frequency.

Pre-asymptotic higher-order methods were devised to solve the above problems by "engineering" the dispersion properties of finite-difference schemes for certain applications [7]-[11]. They start from defining an error functional related to the dispersion property of a given stencil; e.g., the conventional (2,4) stencil [2]. The coefficients of the underlining finite-different scheme are then determined by minimizing this error functional. The criteria can be either minimum dispersion error in a certain angular span or in a certain frequency range. In the former case, one obtains angularly optimized finite-difference schemes [7]-[9]. In the latter case, one obtains so-called Dispersion-Relation-Preserving (DRP) schemes [10]-[11].

An important question arising from the development of pre-asymptotic methods is their truncation error properties. Although they are based on a stencil which is supposed to have a higher-order truncation error, the finite-difference coefficients have been modified for desired numerical dispersion properties. Thus, it is unclear whether the original truncation error properties can be retained.

In order to answer the above question, the truncation error of the Three-Dimensional (3D) DRP scheme, which is based on the (2,4) stencil, is analyzed in this study [11]. This analysis can be adapted to other pre-asymptotic schemes.

II. 3D DRP EQUATIONS

Details of the DRP method can be found in [11]. It is briefly repeated here for convenience. The FDTD discretization of 3D Maxwell's equations in a Cartesian grid by using a (2,4) stencil can be written as:

$$\vec{E}^{i+1}=\vec{E}^{i}+\frac{\Delta t}{\varepsilon}\vec{S}\times\vec{H}^{i+\frac{1}{2}}, \quad (1)$$

$$\vec{H}^{i+\frac{1}{2}}=\vec{H}^{i-\frac{1}{2}}-\frac{\Delta t}{\mu}\vec{S}\times\vec{E}^{i}, \quad (2)$$

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where superscripts indicate time steps. The finite-difference operator $\vec{S}$ is defined as:

$$\vec{S}=\frac{1}{\Delta x}(C_{1x}S_x^{+}+C_{2x}S_x^{++})\hat{x}+\frac{1}{\Delta y}(C_{1y}S_y^{+}+C_{2y}S_y^{++})\hat{y}+\frac{1}{\Delta z}(C_{1z}S_z^{+}+C_{2z}S_z^{++})\hat{z}, \quad (3)$$

where C_{1s} and C_{2s}, s = x, y, z are coefficients to be determined, and S_s^{+} and S_s^{++} are "grid displacement" operators [6] defined by:

$$S_x^{+}E^i_{y_{(l+\frac{1}{2},m+\frac{1}{2},n)}}=E^i_{y_{(l+1,m+\frac{1}{2},n)}}-E^i_{y_{(l,m+\frac{1}{2},n)}}, \quad (4)$$

$$S_x^{++}E^i_{y_{(l+\frac{1}{2},m+\frac{1}{2},n)}}=E^i_{y_{(l+1,m+\frac{1}{2},n)}}-E^i_{y_{(l,m+\frac{1}{2},n)}}, \quad (5)$$

and similarly for the other components. In the above, subscripts indicate spatial locations. By applying standard Fourier analysis, we obtain:

$$\vec{\mathcal{E}}\sin(\frac{\omega\Delta t}{2})=-\frac{\Delta t}{\varepsilon}\vec{F}\times\vec{\mathcal{H}}, \quad (6)$$

$$\vec{\mathcal{H}}\sin(\frac{\omega\Delta t}{2})=\frac{\Delta t}{\mu}\vec{F}\times\vec{\mathcal{E}}, \quad (7)$$

with

$$\vec{F}=F_x\hat{x}+F_y\hat{y}+F_z\hat{z},$$

$$F_x=\frac{1}{\Delta x}[C_{1x}\sin(\frac{k_x\Delta x}{2})+C_{2x}\sin(\frac{3k_x\Delta x}{2})],$$

$$F_y=\frac{1}{\Delta y}[C_{1y}\sin(\frac{k_y\Delta y}{2})+C_{2y}\sin(\frac{3k_y\Delta y}{2})],$$

$$F_z=\frac{1}{\Delta z}[C_{1z}\sin(\frac{k_z\Delta z}{2})+C_{2z}\sin(\frac{3k_z\Delta z}{2})].$$

Considering the H update for the TE^z wave propagating along the (θ, ϕ) direction, its wavenumber components read $k_x = k\sin\theta\cos\phi$, $k_y = k\sin\theta\sin\phi$, $k_z = k\cos\theta$. We have:

$$\mathcal{E}_x=-\mathcal{E}\sin\phi,\ \mathcal{E}_y=\mathcal{E}\cos\phi,\ \mathcal{E}_z=0, \quad (8)$$

$$\mathcal{H}_x=-\mathcal{H}\cos\theta\cos\phi,\ \mathcal{H}_y=-\mathcal{H}\cos\theta\sin\phi,\ \mathcal{H}_z=\mathcal{H}\sin\theta. \quad (9)$$

The following two independent equations can be obtained by substituting (8) and (9) into (7):

$$\mathcal{H}\cos\theta\sin(\frac{\omega\Delta y}{2})=\frac{\Delta t}{\mu\Delta z}[C_{1z}\sin(\frac{k_z\Delta z}{2})+C_{2z}\sin(\frac{3k_z\Delta z}{2})]\mathcal{E}, \quad (10)$$

$$\begin{aligned}\mathcal{H}\sin\theta\sin(\frac{\omega\Delta y}{2})=\frac{\Delta t}{\mu}\{&\frac{1}{\Delta x}\cos\phi[C_{1x}\sin(\frac{k_x\Delta x}{2})+C_{2x}\sin(\frac{3k_x\Delta x}{2})]\\&+\frac{1}{\Delta y}\sin\phi[C_{1y}\sin(\frac{k_y\Delta y}{2})+C_{2y}\sin(\frac{3k_y\Delta y}{2})]\}\mathcal{E}.\end{aligned} \quad (11)$$

The other polarization gives similar equations for the E-field update.

C_{1z} and C_{2z} can be determined from Eqs. (10) and (11). In a regular Cartesian grid, the remaining coefficients can be likewise determined because they obey identical equations with respect to the elevation angles of the associated axes. By enforcing $E=\eta H$, and denoting the Courant-Friedrichs-Levy (CFL) [1] number as $\chi_s=\sqrt{3}v_p\Delta t/\Delta s$, Eq. (10) can be written as:

$$\frac{\sqrt{3}}{\chi_s}\sin(\frac{\pi q_s\chi_s}{\sqrt{3}})\cos\theta=C_{1s}\sin(\pi q_s\cos\theta)+C_{2s}\sin(3\pi q_s\cos\theta), \quad (12)$$

where $q_s=\Delta s/\lambda$ denotes the wavelength to grid-cell size ratio, and Δs stands for either Δx, Δy, or Δz.

An error functional can be defined as the difference between the left- and the right-hand sides of Eq. (12). Expanding it in a series of spherical harmonics $Y_{lm}(\theta, \phi)$ yields:

$$\begin{aligned}\delta(C_{1s},C_{2s},\theta,\phi)=\sum_{l=0}^{\infty}&\sqrt{\pi(4l+3)}[C_{1s}I_{2l+1}(\pi q_s)+C_{2s}I_{2l+1}(3\pi q_s)]\\&Y_{2l+1,0}(\theta,\phi)+\frac{2\sqrt{\pi}}{\chi_s}\sin(\frac{\pi q_s\chi_s}{\sqrt{3}})Y_{1,0}(\theta,\phi),\end{aligned} \quad (13)$$

where $I_l(\alpha) = 0$ for l even. For odd l, $I_l(\alpha)$ can be obtained via integration by parts as:

$$I_l(\alpha)=[\frac{2(2l-3)}{2l-5}-\frac{(2l-1)(2l-3)}{\alpha^2}]I_{l-2}(\alpha)-\frac{2l-1}{2l-5}I_{l-4}(\alpha). \quad (14)$$

The first two terms are given by:

$$I_1(\alpha)=\frac{2(\sin\alpha-\alpha\cos\alpha)}{\alpha^2},$$

$$I_3(\alpha)=\frac{6(2\alpha^2-5)\sin\alpha-2\alpha(\alpha^2-15)\cos\alpha}{\alpha^4}.$$

By enforcing the two leading terms in Eq. (12) to be zero and solving for C_{1s} and C_{2s}, one obtains:

$$C_{1s}=C_{1s}^{(\infty)}\equiv\frac{\pi^2q_s^2[3\pi q_s(5-3\pi^2q_s^2)\cos(3\pi q_s)+(18\pi^2q_s^2-5)\sin(3\pi q_s)]\sin(\frac{\pi q_s\chi_s}{\sqrt{3}})}{\Xi}, \quad (15)$$

$$C_{2s}=C_{2s}^{(\infty)}\equiv\frac{27\pi^2q_s^2[\pi q_s(\pi^2q_s^2-15)\cos(\pi q_s)+3(5-2\pi^2q_s^2)\sin(\pi q_s)]\sin(\frac{\pi q_s\chi_s}{\sqrt{3}})}{\Xi}, \quad (16)$$

where the denominator in Eqs. (15) and (16) writes as:

$$\begin{aligned}\Xi=20\sqrt{3}\chi_s\{&(1+3\pi^2q_s^2)\cos(2\pi q_s)-\cos(4\pi q_s)+\pi q_s\{3\pi q_s[\cos(4\pi q_s)\\&-2\pi q_s\cos(\pi q_s)\sin(\pi q_s)^3]+2[\sin(2\pi q_s)-2\sin(4\pi q_s)]\}\}.\end{aligned}$$

In order to implement these coefficients in time domain, C_{1s}^{∞} and C_{2s}^{∞} can be expanded in a Taylor series around $q_s = 0$. By retaining the lowest order terms and substituting the second order time derivative by the spatial derivative operator $v_p^2\nabla^2$ (from Helmholtz's equation in the continuum), one obtains:

$$C_{1s}^{(2)}=\frac{9}{8}+\frac{1}{64}(\chi_s^2-1)\Delta s^2\nabla^2\equiv C_{11s}^{(2)}-C_{12s}^{(2)}\Delta s^2\nabla^2, \quad (17)$$

$$C_{1s}^{(2)} = -\frac{1}{24} - \frac{1}{1728}(\chi_s^2 - 9)\Delta s^2\nabla^2 \equiv C_{21s}^{(2)} - C_{22s}^{(2)}\Delta s^2\nabla^2 . \quad (18)$$

The final finite-difference scheme is obtained by substituting these coefficients in Eq. (2).

III. TRUNCTION ERROR

Let us consider the H_z update of the DRP scheme in a uniform grid, which is written as:

$$H^{i+\frac{1}{2}}_{z(l+\frac{1}{2},m+\frac{1}{2},n)} = H^{i-\frac{1}{2}}_{z(l+\frac{1}{2},m+\frac{1}{2},n)} + \frac{\Delta t}{\mu}\{\frac{1}{\Delta y}[C_{1y}(E^i_{x(l+\frac{1}{2},m+1,n)} - E^i_{x(l+\frac{1}{2},m,n)}) + C_{2y}(E^i_{x(l+\frac{1}{2},m+2,n)} - E^i_{x(l+\frac{1}{2},m-1,n)})] - \frac{1}{\Delta x}[C_{1x}(E^i_{y(l+1,m+\frac{1}{2},n)} - E^i_{y(l,m+\frac{1}{2},n)}) + C_{2x}(E^i_{y(l+2,m+\frac{1}{2},n)} - E^i_{y(l-1,m+\frac{1}{2},n)})]\}. \quad (19)$$

Plugging Eqs. (17) and (18) into Eq. (19), one obtains:

$$H^{i+\frac{1}{2}}_{z(l+\frac{1}{2},m+\frac{1}{2},n)} = H^{i-\frac{1}{2}}_{z(l+\frac{1}{2},m+\frac{1}{2},n)} + \frac{\Delta t}{\mu}\{\frac{1}{\Delta s}[(\frac{9}{8} + \frac{1}{64}(\chi_s^2 - 1)\Delta s^2\nabla^2)(E^i_{x(l+\frac{1}{2},m+1,n)} - E^i_{x(l+\frac{1}{2},m,n)}) + (-\frac{1}{24} - \frac{1}{1728}(\chi_s^2 - 9)\Delta s^2\nabla^2)(E^i_{x(l+\frac{1}{2},m+2,n)} - E^i_{x(l+\frac{1}{2},m-1,n)})] - \frac{1}{\Delta s}[(\frac{9}{8} + \frac{1}{64}(\chi_s^2 - 1)\Delta s^2\nabla^2)(E^i_{y(l+1,m+\frac{1}{2},n)} - E^i_{y(l,m+\frac{1}{2},n)}) + (-\frac{1}{24} - \frac{1}{1728}(\chi_s^2 - 9)\Delta s^2\nabla^2)(E^i_{y(l+2,m+\frac{1}{2},n)} - E^i_{y(l-1,m+\frac{1}{2},n)})]\}. \quad (20)$$

Note that, the difference between the above update and a conventional (2,4) scheme involves the spatial derivative terms. The time derivative is treated similarly in both approaches, which results in a temporal truncation error of $\mathcal{O}(\Delta t^2)$. So the spatial truncation error will be focused in the following.

Let us consider the spatial derivative term involving E_x only because the E_y term is treated the same as E_x in Eq. (20). One has:

$$\frac{1}{\Delta s}[[\frac{9}{8} + \frac{1}{64}(\chi_s^2 - 1)\Delta s^2\nabla^2](E^i_{x(l+\frac{1}{2},m+1,n)} - E^i_{x(l+\frac{1}{2},m,n)}) + [-\frac{1}{24} - \frac{1}{1728}(\chi_s^2 - 9)\Delta s^2\nabla^2](E^i_{x(l+\frac{1}{2},m+2,n)} - E^i_{x(l+\frac{1}{2},m-1,n)})]. \quad (21)$$

By expanding $E^i_{x(l+\frac{1}{2},m+1,n)}$ in Taylor series as:

$$E^i_{x(l+\frac{1}{2},m+1,n)} = [1 + (\frac{\Delta s}{2})\frac{\partial}{\partial y} + (\frac{\Delta s}{2})^2\frac{1}{2!}\frac{\partial^2}{\partial^2 y} + (\frac{\Delta s}{2})^3\frac{1}{3!}\frac{\partial^3}{\partial^3 y} + (\frac{\Delta s}{2})^4\frac{1}{4!}\frac{\partial^4}{\partial^4 y} + (\frac{\Delta s}{2})^5\frac{1}{5!}\frac{\partial^5}{\partial^5 y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)} + \mathcal{O}(\Delta s^6), \quad (22)$$

and the other terms similarly, it was found that:

$$\frac{1}{\Delta s}[\frac{9}{8}(E^i_{x(l+\frac{1}{2},m+1,n)} - E^i_{x(l+\frac{1}{2},m,n)}) - \frac{1}{24}(E^i_{x(l+\frac{1}{2},m+2,n)} - E^i_{x(l+\frac{1}{2},m-1,n)})] = \frac{\partial}{\partial y}E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)} + \mathcal{O}(\Delta s^4). \quad (23)$$

The remaining term in (21) that needs to be considered is:

$$\frac{1}{\Delta s}[\frac{1}{64}(\chi_s^2 - 1)\Delta s^2\nabla^2(E^i_{x(l+\frac{1}{2},m+1,n)} - E^i_{x(l+\frac{1}{2},m,n)}) - \frac{1}{1728}(\chi_s^2 - 9)\Delta s^2\nabla^2(E^i_{x(l+\frac{1}{2},m+2,n)} - E^i_{x(l+\frac{1}{2},m-1,n)})]. \quad (24)$$

The ∇^2 operators in Eq. (24) are approximated by centered difference; i.e.,

$$\nabla^2 E^i_{x(l+\frac{1}{2},m+1,n)} \approx \frac{1}{\Delta s^2}[E^i_{x(l-\frac{1}{2},m+1,n)} - 2E^i_{x(l+\frac{1}{2},m+1,n)} + E^i_{x(l+\frac{3}{2},m+1,n)}] + \frac{1}{\Delta s^2}[E^i_{x(l+\frac{1}{2},m,n)} - 2E^i_{x(l+\frac{1}{2},m+1,n)} + E^i_{x(l+\frac{1}{2},m+2,n)}] + \frac{1}{\Delta s^2}[E^i_{x(l+\frac{1}{2},m+1,n-1)} - 2E^i_{x(l+\frac{1}{2},m+1,n)} + E^i_{x(l+\frac{1}{2},m+1,n+1)}]. \quad (25)$$

By using Taylor expansion, it is found that:

$$\nabla^2 E^i_{x(l+\frac{1}{2},m+1,n)} = [\frac{\partial^2}{\partial^2 x} + (\Delta s^2)\frac{1}{12}\frac{\partial^4}{\partial^4 x} + \frac{\partial^2}{\partial^2 y} + (\Delta s^2)\frac{1}{12}\frac{\partial^4}{\partial^4 y} + \frac{\partial^2}{\partial^2 z} + (\Delta s^2)\frac{1}{12}\frac{\partial^4}{\partial^4 z}]E^i_{x(l+\frac{1}{2},m+1,n)} + \mathcal{O}(\Delta s^4). \quad (26)$$

By using the following expressions:

$$\frac{\partial^2}{\partial^2 x}E^i_{x(l+\frac{1}{2},m+1,n)} = [\frac{\partial^2}{\partial^2 x} + (\frac{\Delta s}{2})\frac{\partial^3}{\partial^2 x\partial y} + (\frac{\Delta s}{2})^2\frac{\partial^4}{\partial^2 x\partial^2 y} + (\frac{\Delta s}{2})^3\frac{\partial^5}{\partial^2 x\partial^3 y} + (\frac{\Delta s}{2})^4\frac{\partial^6}{\partial^2 x\partial^4 y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)} + \mathcal{O}(\Delta s^5), \quad (27)$$

$$\frac{\partial^4}{\partial^4 x}E^i_{x(l+\frac{1}{2},m+1,n)} = [\frac{\partial^4}{\partial^4 x} + \left(\frac{\Delta s}{2}\right)\frac{\partial^5}{\partial^4 x\partial y} + \left(\frac{\Delta s}{2}\right)^2\frac{\partial^6}{\partial^4 x\partial^2 y} + \left(\frac{\Delta s}{2}\right)^3\frac{\partial^7}{\partial^4 x\partial^3 y} + \left(\frac{\Delta s}{2}\right)^4\frac{\partial^8}{\partial^4 x\partial^4 y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)} + \mathcal{O}(\Delta s^5), \quad (28)$$

one can obtain:

$$\frac{1}{64}(\chi_s^2 - 1)\Delta s^2\nabla^2(E^i_{x(l+\frac{1}{2},m+1,n)} - E^i_{x(l+\frac{1}{2},m,n)}) = \frac{1}{64}(\chi_s^2 - 1)\Delta s^2[(\Delta s)\frac{\partial^3}{\partial^2 x\partial y} + 2\left(\frac{\Delta s}{2}\right)^3\frac{\partial^5}{\partial^2 x\partial^3 y} + (\Delta s)\frac{\partial^3}{\partial^3 y} + 2\left(\frac{\Delta s}{2}\right)^3\frac{\partial^5}{\partial^5 y} + (\Delta s)\frac{\partial^3}{\partial^2 z\partial y} + 2\left(\frac{\Delta s}{2}\right)^3\frac{\partial^5}{\partial^2 z\partial^3 y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)} + \mathcal{O}(\Delta s^5), \quad (29)$$

$$-\frac{1}{1728}(\chi_s^2-9)\Delta s^2\nabla^2(E^i_{x(l+\frac{1}{2},m+2,n)}-E^i_{x(l+\frac{1}{2},m-1,n)})$$
$$=-\frac{1}{1728}(\chi_s^2-9)\Delta s^2[(3\Delta s)\frac{\partial^3}{\partial^2 x\partial y}+2\left(\frac{3\Delta s}{2}\right)^3\frac{\partial^5}{\partial^2 x\partial^3 y}+(3\Delta s)\frac{\partial^3}{\partial^3 y}+$$
$$2\left(\frac{3\Delta s}{2}\right)^3\frac{\partial^5}{\partial^5 y}+(3\Delta s)\frac{\partial^3}{\partial^2 z\partial y}+2\left(\frac{3\Delta s}{2}\right)^3\frac{\partial^5}{\partial^2 z\partial^3 y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)}+\mathcal{O}(\Delta s^5). \quad (30)$$

Thus, (24) becomes:

$$\frac{\chi_s^2}{72}\Delta s^2[\frac{\partial^3}{\partial^2 x\partial y}+\frac{\partial^3}{\partial^3 y}+\frac{\partial^3}{\partial^2 z\partial y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)}+\mathcal{O}(\Delta s^4). \quad (31)$$

Together with Eq. (23), Eq. (21) is written as:

$$\frac{1}{\Delta s}[[\frac{9}{8}+\frac{1}{64}(\chi_s^2-1)\Delta s^2\nabla^2](E^i_{x(l+\frac{1}{2},m+1,n)}-E^i_{x(l+\frac{1}{2},m,n)})+$$
$$[-\frac{1}{24}-\frac{1}{1728}(\chi_s^2-9)\Delta s^2\nabla^2]E^i_{x(l+\frac{1}{2},m+2,n)}-E^i_{x(l+\frac{1}{2},m-1,n)}]$$
$$=\frac{\partial}{\partial y}E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)}+\frac{\chi_s^2}{72}\Delta s^2[\frac{\partial^3}{\partial^2 x\partial y}+\frac{\partial^3}{\partial^3 y}+\frac{\partial^3}{\partial^2 z\partial y}]E^i_{x(l+\frac{1}{2},m+\frac{1}{2},n)}+\mathcal{O}(\Delta s^4). \quad (32)$$

Therefore, the truncation error of the DRP scheme is generally $\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta s^2)$. In the limiting case where the CFL number χ_s goes to zero, the truncation error recovers to $\mathcal{O}(\Delta t^2)+\mathcal{O}(\Delta s^4)$ (from Eq. (32)).

IV. CONCLUSIONS

The truncation error of the DRP scheme was investigated in this study. It serves to reinforce the basic trade-off of pre-asymptotic higher-order finite-difference schemes, which trade low numerical dispersion error at a pre-assigned frequency window or angular range for larger numerical dispersion errors outside the range of interest; in particular, at sufficiently low frequencies where the cumulative numerical dispersion error decreases due to the smaller electrical size. Although higher-order truncation error is not preserved in general, this approach is more relevant to improving the accuracy of practical large-scale simulations of hyperbolic problems, in which the frequency is often limited in a prescribed band.

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