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Corrections to the General (2,4) and (4,4) FDTD Schemes

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Abstract

The sampling weights associated with two general higher order FDTD schemes were derived by Smith, *et al.* and published in a *IEEE Transactions on Antennas and Propagation* article in 2012. Inconsistencies between governing equations and their resulting solutions were discovered within the article. In an effort to track down the root cause of these inconsistencies, the full three-dimensional, higher order FDTD dispersion relation was re-derived using `Mathematica`™. During this process, two errors were identified in the article. Both errors are highlighted in this document. The corrected sampling weights are also provided. Finally, the original stability limits provided for both schemes are corrected, and presented in a more precise form. It is recommended any future implementations of the two general higher order schemes provided in the Smith, *et al.* 2012 article should instead use the sampling weights and stability conditions listed in this document.

1 Background

The Finite-Difference Time Domain (FDTD) method is popular within the computational electromagnetics (CEM) community due to its simplicity, flexibility, and computational efficiency [1, 2]. Most CEM FDTD implementations employ the simplest discretization scheme: second order in time and space (often referred to as the Yee scheme [1]). It can be expressed as (2,2), or second order accurate in time and space, respectively. The Yee scheme approximates both temporal and spatial derivatives using the same, simple centered difference scheme. For example, a spatial derivative of the variable, A, centered at the spatial location, $x_{i+1/2}$, would be approximated as:

$$\left.\frac{\partial A}{\partial x}\right|_{i+1/2} \approx \frac{A_{i+1} - A_i}{x_{i+1} - x_i} \tag{1}$$

For electrically large CEM problems, the Yee scheme can exhibit rather large errors stemming from numerical dispersion and anisotropy. To reduce these errors, *higher order* FDTD schemes may be employed (the trade off often being accuracy for simulation time). Higher order FDTD schemes approximate the same temporal and spatial differentials by simply including more terms.

Two general higher order FDTD schemes were previously developed by Smith, *et al.* [3]. Their higher order stencil requires 36 points (see Figure 1) be sampled when approximating spatial differentials. This is in contrast to the original Yee scheme [1], which itself requires the sampling of only two points (see Figure 1), and the Fang (2,4) FDTD scheme which utilizes only four [4].

2 Error #1: Dispersion Relation

Sampling weights for each of the 36 points in the general (4,4) scheme were again calculated by first re-deriving the full three-dimensional, fourth order FDTD dispersion relation using `Mathematica`™. This is given in its most basic form by:

$$\begin{aligned}\frac{1}{\alpha^2}\mathtt{sin}^2 T = \Big(&\mathtt{sin}x\left[a_{1,0} + 4a_{1,1} + 4a_{1,2} - (4a_{1,1} + 8a_{1,2})\left(\mathtt{sin}^2 y + \mathtt{sin}^2 z\right) + 16a_{1,2}\mathtt{sin}^2 y\mathtt{sin}^2 z\right]\\ &+ \mathtt{sin}3x\left[a_{2,0} + 4a_{2,1} + 4a_{2,2} - (4a_{2,1} + 8a_{2,2})\left(\mathtt{sin}^2 y + \mathtt{sin}^2 z\right) + 16a_{2,2}\mathtt{sin}^2 y\mathtt{sin}^2 z\right]\Big)^2\end{aligned} \tag{2}$$

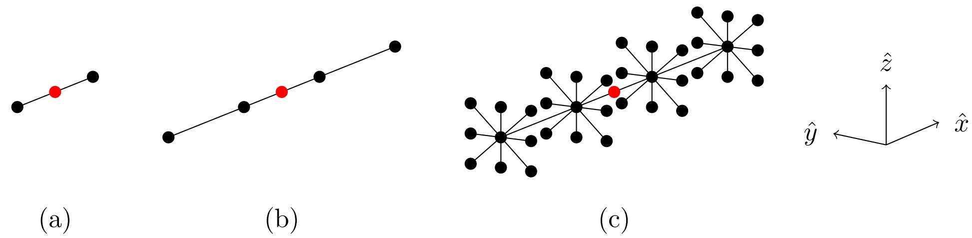

Figure 1: Visual depictions of the (a) Yee, (b) Fang, and (c) General (4,4) spatial discretization schemes for an x-directed derivative as presented [3].

In contrast, Eq (8) of [3] gives this dispersion relation as:

$$\frac{1}{\alpha^2}\texttt{sin}^2 T = \Big(\texttt{sin}x\left[a_{1,0} + 4a_{1,1} + 4a_{1,2} - (4a_{1,1} + 8a_{1,2})\left(\texttt{sin}^2 y + \texttt{sin}^2 z\right) + 32a_{1,2}\texttt{sin}^2 y\texttt{sin}^2 z\right] + \texttt{sin}3x\left[a_{2,0} + 4a_{2,1} + 4a_{2,2} - (4a_{2,1} + 8a_{2,2})\left(\texttt{sin}^2 y + \texttt{sin}^2 z\right) + 32a_{2,2}\texttt{sin}^2 y\texttt{sin}^2 z\right]\Big)^2 \tag{3}$$

The coefficients b_1, b_2, c_1, and c_2 listed in Eq (8) of [3] are not explicitly defined, but may be inferred as:

$$b_1 = a_{1,1} \qquad c_1 = a_{1,2} \qquad b_2 = a_{2,1} \qquad c_2 = a_{2,2}$$

Note the difference (highlighted in red in both equations) between (2) and (3): the leading factors for the last terms in each line (*i.e.* the $a_{m,2}\texttt{sin}^2 y\texttt{sin}^2 z$ terms) are different. That is, the *original* paper uses a factor of 32, while the correct equation requires a factor of 16. This incorrect doubled factor is carried through the rest of the derivation in [3], affecting all following equations, and ultimately the sampling weights themselves. This incorrect doubling of the $a_{m,2}\texttt{sin}^2 y\texttt{sin}^2 z$ terms represents the first error identified in [3].

3 Error #2: Solving for Weights

The second error identified in [3] comes about when solving for the higher order sampling weights. Employing the correct (notwithstanding the first error listed in the previous section) governing equations as given in Eqs (11)-(14), (22), and (26), along with the condition $a_{2,2} = 0$, yields different sampling weights than those listed in Table I of [3]. The reason for this discrepancy between the correct sampling weights and those of Table I is unknown. This incorrect solution of the sampling weights represents the second error identified in [3].

4 Corrected Sampling Weights

The corrected sampling weights for the higher order FDTD schemes are listed here in Table 1. It represents an updated version of Table I from [3]. Although not proven here, substituting the corrected sampling weights listed in Table 1 into Eqs (21) and (28) of [3] does in fact reduce to Eqs (27) and (32) for the general (2,4) and (4,4) schemes, respectively. This same reduction is *not* observed if using the original sampling weights listed in Table I of [3], and is easily verified. Likewise, substituting the original sampling weights from Table I of [3] does *not* yield the conditions given in its Eq (22).

5 Stability

The theoretical maximum Courant-Friedrichs-Lewy (CFL) conditions guaranteeing numerical stability for the various FDTD schemes presented in [3] are listed in its Table II. Specifically, the *Stability* column lists

	Yee (2,2)	Fang (2,4)	General (2,4)	General (4,4)
coefficients	$A_1 + 3A_2 = 1$	$A_1 + 3A_2 = 1$ $A_1 + 27A_2 = 0$ $B_1 + 3B_2 = 0$	$A_1 + 3A_2 = 1$ $A_1 + 27A_2 = 0$ $B_1 + 3B_2 = 0$	$A_1 + 3A_2 = 1$ $A_1 + 27A_2 = \alpha^2$ $B_1 + 3B_2 = \alpha^2/6$
$a_{1,0}$	1	9/8	147/160	147/160-α^2/8
$a_{1,1}$	0	0	39/640	39/640-α^2/96
$a_{1,2}$	0	0	-3/320	-3/320+α^2/96
$a_{2,0}$	0	-1/24	7/480	7/480
$a_{2,1}$	0	0	-9/640	-9/640+α^2/96
$a_{2,2}$	0	0	0	0

Table 1: Correct sampling weights for Yee, Fang, and General (2,4) and (4,4) FDTD schemes. Compare to Table I of [3]. Weights that have changed compared to those given in [3] are highlighted in red.

relative CFL conditions compared to that of the Yee scheme. The stability of any FDTD scheme can be derived from its dispersion relation. For example, the Yee scheme CFL condition in three dimensions is:

$$\Delta t \leq \frac{1}{c} \frac{1}{\sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}} \tag{4}$$

where Δt is the simulation time step, c is the speed of light in vacuum, and Δx, Δy, and Δz are the grid cell widths in the $\hat{x}$-, $\hat{y}$-, and $\hat{z}$-directions, respectively. If $\Delta x = \Delta y = \Delta z$, Eq (4) reduces to:

$$\Delta t \leq \frac{\Delta x}{c\sqrt{3}} \tag{5}$$

Thus, the various factors listed in the *Stability* column of Table II in [3] are all calculated with respect to the Yee scheme CFL factor of $1/\sqrt{3}$.

Upon re-deriving the dispersion relation, the stability conditions for both the general (2,4) and (4,4) schemes were found to be imprecise. Moreover, the correct α-dependence of this condition for the general (4,4) scheme was not present (and thus incorrect). The corrected (and *exact*) stability conditions for the general (2,4) and (4,4) FDTD schemes are provided in Table 2.

Scheme	Stability
general (2,4)	$60\sqrt{6}/113$
general (4,4)	$60\sqrt{6}/(113 - 20\alpha^2)$

Table 2: Correct and *exact* relative CFL conditions (compared to Yee scheme) for higher order FDTD schemes presented in [3]. Note that $\alpha = \nu_p \Delta t/\Delta x$, and is typically set to 0.5.

Note that the exact stability condition for the general (2,4) scheme is approximately 1.3006, or slightly greater than the reported value of 1.3 from [3]. Likewise, the stability condition for the general (4,4) scheme is approximately 1.3608 (for $\alpha = 0.5$), which is again slightly larger than the reported value from [3]. The value of α (typically falling between 0 and 1) affects both the stability condition and sampling weights for the general (4,4) FDTD scheme.

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