# Rigorous Analysis of Numerical Phase and Group Velocity Bounds in Yee's FDTD Grid

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***Abstract*—We present a systematic derivation of the extreme values of phase and group velocity in Yee's finite difference time domain (FDTD) lattice with unequal aspect ratios. Using a Lagrange multiplier based approach, we derive necessary conditions that propagation vector components need to satisfy to attain extreme values in phase and group velocity. A knowledge of these extreme values are useful in designing low numerical dispersion FDTD schemes and also seeding numerical inversion routines of FDTD dispersion relations.**

***Index Terms*—Finite difference time domain (FDTD), group velocity, phase velocity.**

## I. Introduction

PHASE and group velocity anisotropy due to numerical dispersion is one of the major source of errors in standard finite difference time domain (FDTD) schemes [1]. Knowledge of the numerical phase velocity anisotropy help us to design schemes to reduce the numerical dispersion error [2] or to merge analytical propagation results (e.g., plane waves) within the FDTD simulation environment [3].

Schneider *et al.* [4] carried out a detailed theoretical analysis of the bounds of light propagation in one dimensional FDTD grids. They also considered the special case of 3-D propagation in FDTD grids with cubic Yee cells. However, this analysis cannot be easily generalized to 3-D Yee cells with unequal aspect ratios. Taflove and Hagness [1] has provided a qualitative argument and supporting numerical evidence to show that the minimum phase velocity is alligned with the axis which has the largest spatial discretization length. Zhao [5] conjectured about the conditions leading to maximum phase velocity in Yee cells with nonequal aspect ratios and derived an analytical expression for the maximum phase velocity. Zhao [5] also provided detailed numerical analysis to justify the validity of the conjecture leading to the maximum phase velocity.

In this letter, using a Lagrange multiplier based reformulation [6], we rigorously derive analytical expressions for minimum and maximum phase and group velocity bounds in a noncubic Yee FDTD lattice. Our analysis put the empirical results of Taflove *et al.* [1] and Zhao [5] on a firm theoretical ground and also shows a general way to derive similar relations for other nonstandard FDTD methods. Our results for the directions of phase velocity extremum values are much broader than available in the literature [1], [4], [5], but can be shown to reduce to the simplified results of Taflove *et al.* [1] and Zhao [5] under widely used gridding assumptions.

## II. Phase Velocity Bounds

The phase velocity, $v_p$ of a plane wave with angular frequency $\omega$ and propagation constant magnitude $k$ is given by

$$v_p = \frac{w}{k}. \tag{1}$$

We consider the variation of $v_p$ for fixed $\omega$ for different directions of the propagation vector specified using projections $k_x$, $k_y$, and $k_z$ of the propagation vector to $x, y$, and $z$ directions, respectively. Discretization of space using Yee's staggered grid formulation introduces a nonlinear dependency of $k$ with $\omega$ (i.e., dispersion relations) with the following format [1]:

$$\frac{1}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) = \sum_{\zeta\in\{x,y,z\}} \frac{1}{\Delta\zeta^2}\sin^2\left(\frac{k_\zeta\Delta\zeta}{2}\right) \tag{2}$$

where $c$ is the speed of light in vacuum, $\Delta\zeta$ with $\zeta = x, y, z$ are the spatial step sizes and $\Delta t$ is the temporal step size. The stability of the FDTD time stepping is guaranteed if the Courant Factor $S$ is set below unity [1], [5]

$$S = \sqrt{\sum_{\zeta\in\{x,y,z\}} \frac{c^2\Delta t^2}{\Delta\zeta^2}}. \tag{3}$$

When the angular frequency is kept constant, the minimum and maximum values of the phase velocity $v_p$ defined in (1) can be calculated by knowing the minimum ($k_{\min}$) and maximum ($k_{\max}$) values of the propagation constant magnitude. To calculate the $k_{\min}$ and $k_{\max}$ of $k$, we introduce the following Lagrangian:

$$\mathcal{L}(k_\zeta : \zeta\in\{x,y,z\}, \eta_p) = \frac{\eta_p}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) + \sum_{\zeta\in\{x,y,z\}}\left(k_\zeta^2 - \frac{\eta_p}{\Delta\zeta^2}\sin^2\left(\frac{k_\zeta\Delta\zeta}{2}\right)\right) \tag{4}$$

where $\eta_p$ is a Lagrange multiplier [6] that needs to be determined by equating partial derivatives of (4) with respect to $k_x$, $k_y$, $k_z$, and $\eta_p$ to zero. It is interesting to note that (4) is equivalent to $k^2$ regardless of the value of $\eta_p$ because (2) is always

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satisfied for min/max values of $k$. The partial derivative of Lagrangian with respect to the Lagrange multiplier $\eta_p$ recovers (2) where as other variables give the following results:

$$\eta_p \sin(k_\zeta \Delta\zeta) = 2k_\zeta \Delta\zeta \quad \forall\zeta \in \{x,y,z\}. \tag{5}$$

This equation shows that there are three different possibilities that exists for giving extremum values of $k$ as discussed below.

### A. All But One Component of $k_\zeta : \zeta \in \{x,y,z\}$ is Nonzero

Suppose $k_\nu \neq 0$; $\nu \in \{x,y,z\}$ is the nonzero component satisfying (5). Then $k = |k_\nu|$ with $k_\nu$ is calculated using the dispersion relation given in (2)

$$|k_\nu| = \frac{2}{\Delta\nu}\sin^{-1}\left(\frac{\Delta\nu}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right). \tag{6}$$

### B. All But One Component of $k_\zeta : \zeta \in \{x,y,z\}$ is Zero

Suppose $k_\upsilon, k_\kappa \neq 0$; $\upsilon, \kappa \in \{x,y,z\}$ are the nonzero components of the numerical propagation vector. Then from (5), we get the following relation:

$$\mathrm{sinc}(k_\upsilon \Delta\upsilon) = \mathrm{sinc}(k_\kappa \Delta\kappa) \tag{7}$$

where we use the function definition $\mathrm{sinc}(x) = \sin(x)/x$. $\mathrm{sinc}(\zeta)$ is a multiple valued function approximately in the range $[-0.25, 1]$ for $-\infty < \zeta < \infty$. However, the spatial grid should at least have two samples per wavelength to avoid aliasing and hence giving the result:

$$|k_\zeta \Delta\zeta| \leq \pi \quad \forall\zeta \in \{\upsilon,\kappa\} \tag{8}$$

within this range, $\mathrm{sinc}(\zeta)$ function becomes single valued for the absolute value of the argument $\zeta$ (i.e., $|\zeta|$). Using this result, we could solve (7) to get

$$|k_\upsilon|\Delta\upsilon = |k_\kappa|\Delta\kappa. \tag{9}$$

Substituting this result to (2), we get for $\zeta = \upsilon, \kappa$

$$|k_\zeta| = \frac{2}{\Delta\zeta}\sin^{-1}\left(\sin\left(\frac{\omega\Delta t}{2}\right)\Big/\sqrt{\sum_{\zeta\in\{\upsilon,\kappa\}}\frac{c^2\Delta t^2}{\Delta\zeta^2}}\right) \tag{10}$$

noting that $k = (k_\upsilon^2 + k_\kappa^2)^{1/2}$, we get

$$k = \frac{2}{c\Delta t}\sqrt{\sum_{\zeta\in\{\upsilon,\kappa\}}\frac{c^2\Delta t^2}{\Delta\zeta^2}} \times \sin^{-1}\left(\sin\left(\frac{\omega\Delta t}{2}\right)\Big/\sqrt{\sum_{\zeta\in\{\upsilon,\kappa\}}\frac{c^2\Delta t^2}{\Delta\zeta^2}}\right). \tag{11}$$

### C. All the Components of $k_\zeta : \zeta \in \{x,y,z\}$ are Nonzero

In this case, components of the propagation vector simultaneously satisfy the following equalities:

$$\mathrm{sinc}(k_x\Delta x) = \mathrm{sinc}(k_y\Delta y) = \mathrm{sinc}(k_z\Delta z) \tag{12}$$

Using an argument similar to the previous case and using (3), we can easily show $k$ satisfies the following equation:

$$k = \frac{2S}{c\Delta t}\sin^{-1}\left(\frac{1}{S}\sin\left(\frac{\omega\Delta t}{2}\right)\right). \tag{13}$$

### D. Minimum and Maximum Values of $k$

In the previous subsections, we established the possible candidate values that qualify as either minimum or the maximum value of the propagation constant $k$.

Consider the function $\vartheta(\zeta)$ defined in the range $0 \leq \zeta \leq 1$

$$\vartheta(\zeta) = \alpha\sin^{-1}\left(\frac{\zeta}{\alpha}\right) - \beta\sin^{-1}\left(\frac{\zeta}{\beta}\right) \tag{14}$$

where $\alpha$ and $\beta$ are positive constants with $0 < \zeta/\beta \leq \zeta/\alpha \leq 1$. It is straight forward to verify that $\vartheta(0) = 0$ and the derivative of $\vartheta(\zeta)$ with respect to $\zeta$ is positive in the range $0 \leq \zeta \leq 1$. Therefore $\vartheta(\zeta) \geq 0$, giving the following inequality:

$$\alpha\sin^{-1}\left(\frac{\zeta}{\alpha}\right) \geq \beta\sin^{-1}\left(\frac{\zeta}{\beta}\right). \tag{15}$$

Repeated application of inequality (15) to (6), (11) and (13) gives the minimum propagation vector value as

$$k_{\min} = \frac{2S}{c\Delta t}\sin^{-1}\left(\frac{1}{S}\sin\left(\frac{\omega\Delta t}{2}\right)\right) \tag{16}$$

and the maximum value as

$$k_{\max} = \max_{\zeta\in\{x,y,z\}}\left\{\frac{2}{\Delta\zeta}\sin^{-1}\left(\frac{\Delta\zeta}{c\Delta t}\sin\left(\frac{\omega\Delta t}{2}\right)\right)\right\}. \tag{17}$$

## III. Group Velocity Bounds

The group velocity $v_g$ is defined as $v_g = 1/(dk/d\omega)$ [1]. Using the dispersion relation (2), group velocity in standard FDTD grid can be written as

$$v_g = \frac{c^2}{\omega k}\sum_{\zeta\in\{x,y,z\}} k_\zeta^2 \frac{\mathrm{sinc}(k_\zeta\Delta\zeta)}{\mathrm{sinc}(\omega\Delta t)}. \tag{18}$$

It straightforward to see that this expression tends to $c$ when $\Delta\zeta \in \{x,y,z\}$ tend to zero. To calculate the extreme values of $v_g$, we introduce the following Lagrangian:

$$\mathcal{L}_g(k_\zeta : \zeta \in \{x,y,z\}, \eta_g) = \frac{\eta_g}{c^2\Delta t^2}\sin^2\left(\frac{\omega\Delta t}{2}\right) + \sum_{\zeta\in\{x,y,z\}}\left(\frac{c^2k_\zeta^2}{\omega k}\frac{\mathrm{sinc}(k_\zeta\Delta\zeta)}{\mathrm{sinc}(\omega\Delta t)} - \frac{\eta_g}{\Delta\zeta^2}\sin^2\left(\frac{k_\zeta\Delta\zeta}{2}\right)\right) \tag{19}$$

where $\eta_g$ is a Lagrange multiplier [6] that needs to be determined by solving the following set of equations for all $\zeta \in \{x,y,z\}$:

$$\left(\frac{k^2-k_\zeta^2}{k^3}-\frac{\mathrm{sinc}(\omega\Delta t)\eta_g}{2c^2/\omega}\right)\tan(k_\zeta\Delta\zeta)+\frac{k_\zeta\Delta\zeta}{k}=0. \quad (20)$$

It is easy to show that these equations are satisfied by all but one component of $k_\zeta : \zeta \in \{x,y,z\}$ is nonzero. Using a similar approach as that for extremes of phase velocity, we can then derive the following expression for the minimum value of the group velocity:

$$(v_g)_{\min}=\min_{\nu\in\{x,y,z\}}\left\{\frac{c^2\sin(|k_\nu|\Delta\nu)}{\omega\Delta\nu\,\mathrm{sinc}(\omega\Delta t)}\right\} \quad (21)$$

where $k_\nu \in \{x,y,z\}$ are given in (6). For these $k_\nu$ values, noting that $|k_\alpha|\mathrm{sinc}(|k_\alpha|\Delta\alpha) < |k_\beta|\mathrm{sinc}(|k_\beta|\Delta\beta)$ when $\Delta\alpha > \Delta\beta$, $|k_\alpha|\Delta\alpha < \pi$ and $|k_\beta|\Delta\beta < \pi$ where $\alpha$, $\beta \in \{x,y,z\}$, it is possible to conclude similar to phase velocity, group velocity attains its minimum value along the axis with largest spatial discretization length.

The maximum group velocity results when none of the $k_\zeta \in \{x,y,z\}$ components are zero. Then (20) can be rearranged to get the following simultaneous equations for all $\alpha$, $\beta \in \{x,y,z\}$:

$$\frac{k_\alpha\Delta\alpha}{\tan(k_\alpha\Delta\alpha)}-\frac{k_\alpha^2}{k^2}=\frac{k_\beta\Delta\beta}{\tan(k_\beta\Delta\beta)}-\frac{k_\beta^2}{k^2}. \quad (22)$$

For cubic Yee cells with size $\Delta\ell$, we could solve this equation because all the propagation-constant projections $k_\zeta \in \{x,y,z\}$ are equal to $k_{\Delta\ell}$ and thus falling along the diagonals of the cubic cells

$$k_{\Delta\ell}=\frac{2}{\Delta\ell}\sin^{-1}\left(\frac{1}{S}\sin\left(\frac{\omega\Delta\ell S}{2\sqrt{3}c}\right)\right). \quad (23)$$

However, when the aspect ratios are not equal, it is not possible to solve this equation analytically. Suppose $\Delta\zeta = (1+\epsilon_\zeta)\Delta\ell$ with $|\epsilon_\zeta| \ll 1$ for all $\zeta \in \{x,y,z\}$. Then, we could derive from (22) the following approximate equations for the projections of the propagation constants:

$$k_\zeta \approx k_{\Delta\ell}\left(1-\left(\frac{\varphi(\Delta z,k_{\Delta\ell})k_{\Delta\ell}\Delta\ell}{2/3+\varphi(k_{\Delta\ell},\Delta\ell)k_{\Delta\ell}\Delta\ell}\right)\epsilon_\zeta\right) \quad (24)$$

where $\varphi(\alpha,\beta)$ is a positive function with the following definition:

$$\varphi(\alpha,\beta)=\frac{2\alpha-\sin(2\alpha\beta)}{1-\cos(2\alpha\beta)}. \quad (25)$$

We can calculate the maximum value of group velocity by substituting these values to (18).

Also consider the ratio of phase velocity to group velocity

$$\frac{v_g}{v_p}=\frac{c^2}{\omega^2}\sum_{\zeta\in\{x,y,z\}}k_\zeta^2\frac{\mathrm{sinc}(k_\zeta\Delta\zeta)}{\mathrm{sinc}(\omega\Delta t)}. \quad (26)$$

Similar to the previous cases, we could introduce a Lagrangian with the dispersion relation constant (2) to derive the following results at the optimum point:

$$\frac{k_x\Delta x}{\tan(k_x\Delta x)}=\frac{k_y\Delta y}{\tan(k_y\Delta y)}=\frac{k_z\Delta z}{\tan(k_z\Delta z)}. \quad (27)$$

Within in the constraints $|k_\zeta\Delta\zeta \le \pi$ for all $\zeta \in \{x,y,z\}$ above equations reduce to $k_x\Delta x = k_y\Delta y = k_z\Delta z$. Noting that this condition leads to the minimum propagation vector $k_{\min}$ given by (16), we get the following inequality for (26):

$$\frac{v_g}{v_p}\le\frac{c^2}{\omega^2 k_{\min}^2}=\frac{c^2}{\left((v_p)_{\max}\right)^2}. \quad (28)$$

Thus, giving the following upper bound for the group velocity maximum:

$$(v_g)_{\max}\le\frac{c^2}{(v_p)_{\max}}. \quad (29)$$

## IV. Conclusion

Using a systematic formulation, we derived the bounds of phase and group velocity in standard Yee latices with unequal aspect ratios using the Lagrange multiplier based approach. Our method can be easily generalized to other staggered-grid time-stepping techniques for Maxwell's equations and also provides the ability to determine seeding guesses for numerical inversion of dispersion relations in Yee lattices. Also, our analysis put the empirical results of Taflove *et al.* [1] and Zhao [5] on a firm theoretical ground. Our results for the directions of phase velocity extremum values are much broader than available in the literature [1], [4], [5], but can be shown to reduce to simplified results of Taflove *et al.* [1] and Zhao [5] under widely used gridding assumptions.

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