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Stability and dispersion analysis of high order FDTD methods for Maxwell's equations in dispersive media

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Abstract. Based on recent work (Bokil, Gibson, 2012) that derived a concise formula for the symbol of spatial high order finite difference approximations of first order differential operators, we analyze the stability and dispersion properties of second order accurate in time and $2M, M > 1$ order accurate in space finite difference schemes for Maxwell's equations in dispersive media of Debye type in two dimensions.

1. Introduction

Computational methods for electromagnetic interrogation problems must be highly efficient, consistent and stable. Simulations are used in critical applications such as cancer detection and explosives characterization [**1**]. Many important materials exhibit dielectric dispersion. Thus, an appropriate discretization method should have a numerical dispersion that matches the model dispersion as closely as possible. Common models of dispersive materials include the Debye model for orientational polarization [**5**] and the Lorentz model for electronic polarization [**1**].

We derive stability conditions and demonstrate numerical dispersion error for arbitrary (even) order in space and second order in time finite difference time domain (FDTD) schemes for Maxwell's equations in two dimensions coupled to Debye polarization models via an auxilliary differential equation (ADE) approach [**4**, **7**]. The work here is an extension of the effort in [**3**] where results were obtained for dispersive Maxwell's equations reduced to one spatial dimension based on work done in [**2**, **7**] for the second order Yee FDTD scheme [**8**]. Stability and dispersion analysis for the Yee FDTD scheme applied to Maxwell's equations coupled with different dispersive models such as Debye and Lorentz polarization models, with the ADE approach, in two and three dimensions can be found in [**2**, **7**].

The key result required to perform the stability and dispersion analyses for arbitrary (even) order $2M, M \in \mathbb{N}$ spatial discretizations is the equivalence of the symbol of the $2M$ order finite difference approximation of the first order derivative operator $\partial/\partial z$ with the truncation of an appropriate series expansion of the symbol of $\partial/\partial z$ [**3**].

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2. Model Formulation

Making the assumption that no fields exhibit variation in the z direction, we consider the Maxwell curl equations in two dimensions (the TE mode), which govern the electric field $\mathbf{E}$, and the magnetic field $\mathbf{H}$ in a domain Ω with no free charges in the time interval $(0, T)$, given as

$$\frac{\partial B}{\partial t} = -\text{curl } \mathbf{E}, \tag{2.1a}$$

$$\frac{\partial \mathbf{D}}{\partial t} = \frac{1}{\mu_0}\mathbf{curl}\ B, \tag{2.1b}$$

where $\text{curl } \mathbf{U} = \frac{\partial U_y}{\partial x} - \frac{\partial U_x}{\partial y}$ is the scalar curl operator and $\mathbf{curl}\ U = \left(\frac{\partial U}{\partial y}, -\frac{\partial U}{\partial x}\right)^T$ is the vector curl operator in two dimensions [**6**]. The fields of interest are $B = B_z$, $\mathbf{E} = (E_x, E_y)^T$, and $\mathbf{D} = (D_x, D_y)^T$. The fields $\mathbf{D}, \mathbf{B}$ are the electric, and magnetic flux densities, respectively. All the fields in (2.1) are functions of position $\mathbf{x} = (x, y)$ and time t. We neglect the effects of boundary conditions and initial conditions.

We will consider the case of a dispersive dielectric medium in which magnetic effects are negligible. The dispersive dielectric is modeled as a single-pole Debye medium exhibiting orientational polarization [**4**, **5**]. Thus, within the dielectric medium we have constitutive relations that relate the flux densities $\mathbf{D}, \mathbf{B}$ to the electric, and magnetic fields, respectively, as

$$\tau\frac{\partial \mathbf{D}}{\partial t} + \mathbf{D} = \epsilon_0\epsilon_\infty\tau\frac{\partial \mathbf{E}}{\partial t} + \epsilon_0\epsilon_s\mathbf{E}, \tag{2.2a}$$

$$\mathbf{B} = \mu_0\mathbf{H}. \tag{2.2b}$$

The parameters ϵ_0, and μ_0, are the permittivity, and permeability, respectively, of free space. In equation (2.2a), the parameter ϵ_s is the static relative permittivity and τ is the relaxation time of the Debye medium. The presence of instantaneous polarization is accounted for by the coefficient ϵ_∞, the infinite frequency permittivity, in the Debye model (2.2a) [**1**]. We will call the Maxwell's equations (2.1) coupled with the constitutive laws (2.2) as the *Maxwell-Debye* model.

3. High Order Numerical Methods for Dispersive Media

In this section we construct a family of finite difference schemes for the Maxwell-Debye model (2.1)-(2.2). These schemes are based on the discrete higher order $(2M,\ M \in \mathbb{N})$ approximations $\mathcal{D}^{(2M)}_{\Delta w}$, to the first order spatial differential operator $\partial/\partial w, w = x, y,$ or z, that were constructed in [**3**]. For the time discretization we employ the standard leap-frog scheme which is second order accurate in time. We will denote the resulting schemes as $(2, 2M)$ schemes. When $M = 1$, the corresponding $(2, 2)$ schemes are extensions of the famous Yee scheme [**8**] or FDTD scheme for Maxwell's equations to dispersive media.

Let us denote the time step by $\Delta t > 0$ and the spatial mesh step sizes in the x and y directions by $\Delta x > 0$, and $\Delta y > 0$, respectively. The high order FDTD schemes described here utilize, like the Yee scheme, staggering in space and time of the components of the electric field and flux density with the magnetic field and flux density. We define $t^n = n\Delta t$, $x_\ell = \ell\Delta x$ and $y_j = j\Delta y$, for $n, \ell, j \in \mathbb{Z}$. We also define staggered nodes in the time direction and the x and y direction, respectively as $t^{n+\frac{1}{2}} = t^n + \frac{1}{2}\Delta t$, $x_{\ell+\frac{1}{2}} = x_\ell + \frac{1}{2}\Delta x$, and $y_{j+\frac{1}{2}} = y_j + \frac{1}{2}\Delta y$. The components E_x, D_x of the electric field and electric flux density are discretized at nodes $(t^n, x_{\ell+\frac{1}{2}}, y_j)$, whereas the components E_y, D_y are discretized at nodes $(t^n, x_\ell, y_{j+\frac{1}{2}})$ in the space-time mesh. Finally, the component B of the magnetic flux density is discretized at nodes $(t^{n+\frac{1}{2}}, x_{\ell+\frac{1}{2}}, y_{j+\frac{1}{2}})$. For any field variable $V(t,x,y)$, we denote the approximation of $V(t^n, x_\ell, y_j)$ by $V^n_{\ell,j}$ on the space-time mesh. With the above notation, the $(2,2M)$ discretized schemes for the two dimensional Maxwell-Debye system given in (2.1)-(2.2) are

(3.1a)
$$\frac{B^{n+\frac{1}{2}}_{\ell+\frac{1}{2},j+\frac{1}{2}} - B^{n-\frac{1}{2}}_{\ell+\frac{1}{2},j+\frac{1}{2}}}{\Delta t} = \sum_{p=1}^{M} \frac{\lambda^{2M}_{2p-1}}{(2p-1)\Delta y}\left(E^n_{x_{\ell+\frac{1}{2},j+p}} - E^n_{x_{\ell+\frac{1}{2},j-p+1}}\right) - \sum_{p=1}^{M} \frac{\lambda^{2M}_{2p-1}}{(2p-1)\Delta x}\left(E^n_{y_{\ell+p,j+\frac{1}{2}}} - E^n_{y_{\ell-p+1,j+\frac{1}{2}}}\right),$$

$$\text{(3.1b)} \quad \frac{D^{n+1}_{x_{\ell+\frac{1}{2},j}} - D^n_{x_{\ell+\frac{1}{2},j}}}{\Delta t} = \frac{1}{\mu_0}\sum_{p=1}^{M} \frac{\lambda^{2M}_{2p-1}}{(2p-1)\Delta y}\left(B^{n+\frac{1}{2}}_{\ell+\frac{1}{2},j+p-\frac{1}{2}} - B^{n+\frac{1}{2}}_{\ell+\frac{1}{2},j-p+\frac{1}{2}}\right),$$

$$\text{(3.1c)} \quad \frac{D^n_{y_{\ell,j+\frac{1}{2}}} - D^n_{y_{\ell,j+\frac{1}{2}}}}{\Delta t} = -\frac{1}{\mu_0}\sum_{p=1}^{M} \frac{\lambda^{2M}_{2p-1}}{(2p-1)\Delta x}\left(B^{n+\frac{1}{2}}_{\ell+p-\frac{1}{2},j+\frac{1}{2}} - B^{n+\frac{1}{2}}_{\ell-p+\frac{1}{2},j+\frac{1}{2}}\right),$$

where
$$\lambda^{2M}_{2p-1} = \frac{2(-1)^{p-1}[(2M-1)!!]^2}{(2M+2p-2)!!(2M-2p)!!(2p-1)},$$
as given in [**3**], and the double factorial is defined as
$$n!! = \begin{cases} n\cdot(n-2)\cdot(n-4)\ldots 5\cdot 3\cdot 1 & n>0, \text{ odd} \\ n\cdot(n-2)\cdot(n-4)\ldots 6\cdot 4\cdot 2 & n>0, \text{ even} \\ 1, & n=-1,0. \end{cases}$$

For a Debye media we add the discretized (second order finite difference in time) version of the equation (2.2a) to the discrete scheme defined in (3.1). The discretization of equation (2.2a) in scalar form is

$$\text{(3.2a)} \quad \epsilon_0\epsilon_\infty\tau\frac{E^{n+1}_{x_{\ell+\frac{1}{2},j}} - E^n_{x_{\ell+\frac{1}{2},j}}}{\Delta t} + \epsilon_0\epsilon_s\frac{E^{n+1}_{x_{\ell+\frac{1}{2},j}} + E^n_{x_{\ell+\frac{1}{2},j}}}{2} = \tau\frac{D^{n+1}_{x_{\ell+\frac{1}{2},j}} - D^n_{x_{\ell+\frac{1}{2},j}}}{\Delta t} + \frac{D^{n+1}_{x_{\ell+\frac{1}{2},j}} + D^n_{x_{\ell+\frac{1}{2},j}}}{2},$$

$$\text{(3.2b)} \quad \epsilon_0\epsilon_\infty\tau\frac{E^{n+1}_{y_{\ell,j+\frac{1}{2}}} - E^n_{y_{\ell,j+\frac{1}{2}}}}{\Delta t} + \epsilon_0\epsilon_s\frac{E^{n+1}_{y_{\ell,j+\frac{1}{2}}} + E^n_{y_{\ell,j+\frac{1}{2}}}}{2} = \tau\frac{D^{n+1}_{y_{\ell,j+\frac{1}{2}}} - D^n_{y_{\ell,j+\frac{1}{2}}}}{\Delta t} + \frac{D^{n+1}_{y_{\ell,j+\frac{1}{2}}} + D^n_{y_{\ell,j+\frac{1}{2}}}}{2},$$

4. Stability Analysis

To determine stability conditions we use von Neumann analysis which allows us to localize roots of certain classes of polynomials [**2**]. We follow the approach in [**2**] in which the author derives stability conditions for the $(2,2)$ (Yee) schemes applied to Debye and Lorentz dispersive media. This analysis is based on properties of Schur and von Neumann polynomials.

Stability conditions for the general $(2,2M)$ schemes are made possible by the results presented in [**3**], in which $2M$ order finite difference approximations $\mathcal{D}^{(2M)}_{\Delta w}$, of the first order derivative operator $\partial/\partial w, w = x, y, z$, are described in terms of a truncation of a series expansion of the symbol of this operator

$$\mathcal{F}\left(\mathcal{D}^{(2M)}_{\Delta w}\right) = \frac{2i}{\Delta w}\sum_{p=1}^{M} \gamma_{2p-1}\sin^{2p-1}(k_w \Delta w/2), \tag{4.1}$$

with $\gamma_{2p-1} = \dfrac{[(2p-3)!!]^2}{(2p-1)!}$, and k_w is the component of the wave vector in the $w = x, y$ or z dimension. In performing the von Neumann analysis for the $(2,2M)$ schemes we show that the resulting amplification matrices retain the same structure as in the $(2,2)$ schemes in [**2**], albeit with a generalized definition of the parameter q in [**2**] that appears in this matrix.

4.1. Stability Analysis for $(2,2M)$ Schemes for Debye Media. We consider the $(2,2M)$ scheme for discretizing Maxwell's equations coupled with the Debye polarization model presented in the form of equations (3.1) and (3.2a).

We assume a spatial dependence of the following form in the field quantities

$$\begin{aligned} &B^{n-\frac{1}{2}}_{\ell+\frac{1}{2},j+\frac{1}{2}} = \hat{B}^{n-\frac{1}{2}}(k_x,k_y)\mathrm{e}^{\mathrm{i}k_x x_{\ell+\frac{1}{2}}+\mathrm{i}k_y y_{j+\frac{1}{2}}};\\ &E^n_{x_{\ell+\frac{1}{2},j}} = \hat{E}^n_x(k_x,k_y)\mathrm{e}^{\mathrm{i}k_x x_{\ell+\frac{1}{2}}+\mathrm{i}k_y y_j}; \quad E^n_{y_{\ell,j+\frac{1}{2}}} = \hat{E}^n_y(k_x,k_y)\mathrm{e}^{\mathrm{i}k_x x_\ell+\mathrm{i}k_y y_{j+\frac{1}{2}}};\\ &D^n_{x_{\ell+\frac{1}{2},j}} = \hat{D}^n_x(k_x,k_y)\mathrm{e}^{\mathrm{i}k_x x_{\ell+\frac{1}{2}}+\mathrm{i}k_y y_j}; \quad D^n_{y_{\ell,j+\frac{1}{2}}} = \hat{D}^n_y(k_x,k_y)\mathrm{e}^{\mathrm{i}k_x x_\ell+\mathrm{i}k_y y_{j+\frac{1}{2}}}; \end{aligned} \tag{4.2}$$

with $k_w, w = x, y$, the component of the wave vector $\mathbf{k}$ in the w dimension, i.e. $\mathbf{k} = (k_x, k_y)^T$. The wave number is $k = \sqrt{k_x^2 + k_y^2}$. We define the vector

$$\mathbf{U}^n := [c_\infty \hat{B}^{n-\frac{1}{2}},\ \hat{E}^n_x,\ \frac{1}{\epsilon_0\epsilon_\infty}\hat{D}^n_x,\ \hat{E}^n_y,\ \frac{1}{\epsilon_0\epsilon_\infty}\hat{D}^n_y]^T. \tag{4.3}$$

Substituting the forms (4.2) into the higher order schemes (3.1) and (3.2a), and canceling out common terms we obtain the system $\mathbf{U}^{n+1} = \mathcal{A}\mathbf{U}^n$, where the amplification matrix $\mathcal{A}$ is

$$\begin{bmatrix} 1 & \sigma_y & 0 & -\sigma_x & 0 \\ -\sigma_y^*\theta^+ & \tilde{\theta} - q_y\theta^+ & \theta^+ - \theta^- & \sigma_y^*\sigma_x\theta^+ & 0 \\ -\sigma_y^* & -q_y & 1 & \sigma_y^*\,\sigma_x & 0 \\ \sigma_x^*\theta^+ & \sigma_x^*\sigma_y\theta^+ & 0 & \tilde{\theta} - q_x\theta^+ & \theta^+ - \theta^- \\ \sigma_x^* & \sigma_x^*\sigma_y & 0 & -q_x & 1 \end{bmatrix}.$$

In the above, we have used the following simplifying notation

$$\tilde{\theta} := \frac{2 - h_\tau \epsilon_q}{2 + h_\tau \epsilon_q}, \quad \theta^+ := \frac{2 + h_\tau}{2 + h_\tau \epsilon_q}, \quad \theta^- := \frac{2 - h_\tau}{2 + h_\tau \epsilon_q}.$$

For $w = x, y$, we define the parameter $\eta_w := (c_\infty \Delta t)/\Delta w$, where the parameter $c_\infty^2 := 1/(\epsilon_0 \mu_0 \epsilon_\infty) = c_0^2/\epsilon_\infty$. The speed of light in vacuum is donoted by c_0, and c_∞ is the maximum speed of light in the Debye medium. We note that each parameter, η_x and η_y, is a Courant (stability) number. Other parameters are defined as $h_\tau := \Delta t/\tau$ and $\epsilon_q := \epsilon_s/\epsilon_\infty$ with $\epsilon_s > \epsilon_\infty$ (i.e., $\epsilon_q > 1$) and $\tau > 0$. In the above, the parameter $q_w, w = x, y$ is defined to be $q_w := \sigma_w \sigma_w^*$ [**3**] with

$$\sigma_w := -\eta_w \Delta w \mathcal{F}\left(\mathcal{D}_{\Delta w}^{(2M)}\right) \tag{4.4}$$

and $\sigma_w^* = -\sigma_w$ is the complex conjugate of σ_w. We utilize the description of the symbol of the discrete operator $\mathcal{F}\left(\mathcal{D}_{\Delta w}^{(2M)}\right)$ given in (4.1) to evaluate in terms of k_w and Δw only.

Now, using the results of the von Neumann stability analysis performed in [**2**], we can generalize the stability analysis of the Yee scheme to the $(2, 2M)$ schemes. From the assumption $\epsilon_s > \epsilon_\infty$, a necessary and sufficient stability condition for the $(2, 2M)$ schemes in (3.1) and (3.2a) is that $q := q_x + q_y \in (0, 4)$, for all wave vector components, k_x and k_y [**2**], i.e.,

$$4\eta_x^2 \left(\sum_{p=1}^{M} \gamma_{2p-1} \sin^{2p-1}\left(\frac{k_x \Delta x}{2}\right)\right)^2 + 4\eta_y^2 \left(\sum_{p=1}^{M} \gamma_{2p-1} \sin^{2p-1}\left(\frac{k_y \Delta y}{2}\right)\right)^2 < 4, \ \forall k_w, \tag{4.5}$$

$w = x, y$, which implies that

$$\Delta t < \frac{1}{\left(\sum_{p=1}^{M} \frac{[(2p-3)!!]^2}{(2p-1)!}\right) c_\infty \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}. \tag{4.6}$$

In the limiting case (as $M \to \infty$), we may evaluate the infinite series using results in [**3**]. The positivity of the coefficients γ_{2p-1} implies that the following constraint guarantees stability for all orders in two dimensions

$$\Delta t < \frac{2}{\pi c_\infty \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2}}}. \tag{4.7}$$

5. Dispersion Analysis

As mentioned in the introduction, the models for dispersive media have actual physical dispersion which needs to be modeled correctly. In this section we construct the numerical dispersion relations for the $(2, 2M)$ schemes presented in (3.1)-(3.2). We plot the phase error using representative values for all the parameters of the model.

A plane wave solution of the continuous Maxwell-Debye model (2.1)-(2.2) gives us the following (exact) dispersion relation

$$k_{\mathrm{EX}}^{\mathrm{D}}(\omega) = \frac{\omega}{c}\sqrt{\epsilon_r^{\mathrm{D}}(\omega)}; \quad \epsilon_r^{\mathrm{D}}(\omega) := \frac{\epsilon_s \lambda - i\omega \epsilon_\infty}{\lambda - i\omega}. \tag{5.1}$$

In the above, $\epsilon_r^{\mathrm{D}}(\omega)$ is the relative complex permittivity of the Debye medium, $\lambda := 1/\tau$ and ω is the angular frequency of the plane wave, and $k_{\mathrm{EX}}^{\mathrm{D}}(\omega)$ is the corresponding wave number.

By considering plane wave solutions for all the discrete variables in the $(2, 2M)$ finite difference schemes for the Maxwell-Debye system given in (3.1)-(3.2), we can derive the numerical dispersion relation of this scheme. The numerical dispersion relations of the $(2, 2M)$ schemes (3.1)-(3.2), for the Maxwell-Debye model, are given implicitly by

$$\left|\mathcal{F}\left(\mathcal{D}_{\Delta x}^{(2M)}\right)\right|^2 + \left|\mathcal{F}\left(\mathcal{D}_{\Delta y}^{(2M)}\right)\right|^2 = \frac{\omega_\Delta^2}{c^2}\left(\frac{\epsilon_s\lambda_\Delta - \mathrm{i}\omega_\Delta\epsilon_{\infty,\Delta}}{\lambda_\Delta - \mathrm{i}\omega_\Delta}\right),$$

where the parameters

$$\epsilon_{\infty,\Delta} := \epsilon_\infty; \quad \lambda_\Delta := \lambda\cos(\omega\Delta t/2), \tag{5.2}$$

are discrete representations of the corresponding continuous model parameters. In addition the parameter ω_Δ, which is a discrete representation of the frequency, is defined as

$$\omega_\Delta := \omega\frac{\sin(\omega\Delta t/2)}{\omega\Delta t/2}. \tag{5.3}$$

We define the phase error Φ for a method applied to a particular model to be

$$\Phi = \left|\frac{k_{\mathrm{EX}} - k_{\Delta,M}}{k_{\mathrm{EX}}}\right|, \tag{5.4}$$

where the numerical wave number $k_{\Delta,M}$ is implicitly determined by the corresponding dispersion relation and k_{EX} is the exact wave number. The components of the wave vector are $k_x = \mathbf{k}\cos(\theta)$ and $k_y = \mathbf{k}\sin(\theta)$, where θ is the angle made by the incident plane wave with the horizontal.

To generate the plots below we have assumed the following values of the physical parameters:

$$\epsilon_\infty = 1; \quad \epsilon_s = 78.2; \quad \tau = 8.1\times 10^{-12}\ \mathrm{sec}. \tag{5.5}$$

These are appropriate constants for modeling water and are representative of a large class of Debye type materials [**1**]. In order to resolve all the time scales, the time step is determined by the choice of h_τ via $\Delta t = h_\tau\tau$, and consequently the spatial step $\Delta := \Delta x = \Delta y$ is chosen based on the CFL number $\eta := \eta_x = \eta_y = c_\infty\Delta t/\Delta$.

In the plots of Figure 1 we depict graphs of the phase error Φ, versus frequency ω, for the $(2, 2M)$th order finite difference methods applied to the Maxwell-Debye model in two dimensions, as given in equations (3.1) and (3.2a), for (spatial) orders $2M = 2, 4, 6, 8$ and the limiting $(M = \infty)$ case. The temporal refinement factor, $h_\tau = \Delta t/\tau$, is fixed at 0.1. The plots use values of η set to the maximum stable value for the order, as given in (4.6). We see that increasing θ to $\pi/4$ decreases the phase error, but that the effect is lessened for smaller frequencies and increasing orders. The graphs corresponding to each angle converge to nearly the one dimensional result for the given h_τ and order (it converges nearby and not to the 1D result because the CFL condition for 2D is more restrictive and we are using the highest stable CFL number). With $h_\tau = 0.01$ the graphs corresponding to various angles converge at order 4 (plot not shown). Regardless of angle, for the frequencies of interest (i.e., those near $\omega\tau = 1$), the higher order methods exhibit a gradual improvement over the second order method.

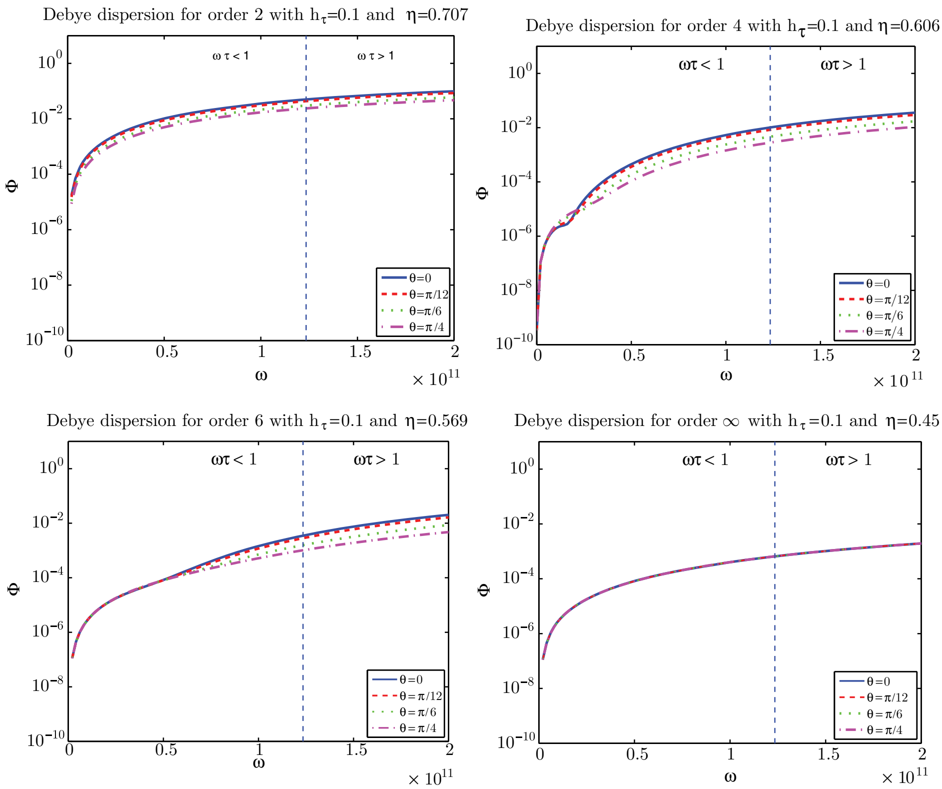

FIGURE 1. Semi-log plots of phase error versus frequency ω for various orders using the largest stable CFL number (η). The vertical line depicts $\omega\tau = 1$. Several angles (θ) are demonstrated.

In Figure 2 we show polar plots of the phase error on a log axis (i.e., the exponent is labeled in the radial dimension). In these plots $\omega = 1/\tau$ and $h_\tau = 0.1$ (left) and $h_\tau = 0.01$ (right). We again see the lessening effect of angle (θ) as the order increases. Further, as in the one dimensional case [**3**], we observe orders of magnitude decreases in Φ as h_τ is decreased. The right plot in particular supports the argument that fourth order is sufficient for minimizing phase error. Any additional decrease in error due to the accuracy of the method is countered by the stability constraint requiring a relatively larger spatial step (Δ).

6. Conclusions

Necessary and sufficient stability conditions, explicitly dependent on the material parameters and the order of the discrete scheme, are presented for Maxwell's equations in Debye dispersive media in two spatial dimensions. Bounds for stability for all orders are obtained by computing the limiting (infinite order) case. We have derived a concise representation of the numerical dispersion relation for each scheme of arbitrary order, which allows an efficient method for predicting the numerical characteristics of a simulation of electromagnetic wave propagation in a dispersive material. This analysis can be extended to higher order discrete schemes

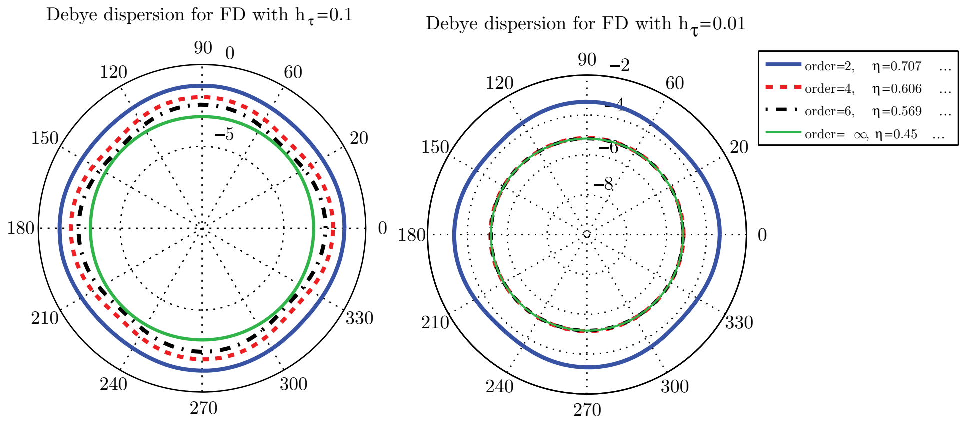

FIGURE 2. Polar semi-log plot of dispersion error versus angle θ for various orders with $h_\tau = 0.1$ (left) and $h_\tau = 0.01$ (right).

for other types of dispersive materials such as Lorentz or Drude media. One can similarly extend the results to three dimensions, however the details are tedious [**2**].

Acknowledgments

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