Analysis of High Order FDTD Methods For Maxwell's Equations in Dispersive Media

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Abstract

The stability properties, and the phase error present in higher order (in space) staggered finite difference schemes for Maxwell's equations coupled with a Debye polarization model are analyzed. We present a novel expansion of the symbol of finite difference approximations, of arbitrary (even) order, of the first order spatial derivative operator. This representation allows the derivation of a closed-form analytical stability condition for all (even) order schemes, including the limiting (infinite order) case. We further derive a concise formula for the numerical dispersion relation.

Introduction

Computational simulations of the propagation and scattering of transient electromagnetic waves in dispersive dielectrics can be studied by numerically solving the time-dependent Maxwell's equations coupled to equations that describe the evolution of the induced macroscopic polarization [1]. The latter incorporates the physical dispersion of the medium and its response to the electromagnetic pulse.

We consider Maxwell's equations in Debye dispersive media using the auxilliary differential equation (ADE) approach, and analyze high order (in space) staggered (Yee) FDTD-like methods for the numerical discretization of the augmented Maxwell system. Our focus in this paper is the derivation of closed form analytical stability criteria for high order staggered finite difference methods including the limiting infinite order method. In addition we also derive numerical dispersion relations for these schemes.

1 Model Formulation

We consider the Maxwell curl equations, 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

$$\frac{\partial \mathbf{D}}{\partial t} - \frac{1}{\mu_0}\nabla \times \mathbf{B} = \mathbf{0} \text{ in } (0,T)\times\Omega, \tag{1.1a}$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = \mathbf{0} \text{ in } (0,T)\times\Omega, \tag{1.1b}$$

along with initial conditions. The fields $\mathbf{D}, \mathbf{B}$ are the electric, and magnetic flux densities, respectively. All the fields in (1.1) are functions of position $\mathbf{x} = (x, y, z)$ and time t. Here we neglect the effects of boundary conditions.

We will consider the case of a dispersive dielectric medium in which magnetic effects are negligible. 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

$$\mathbf{D} = \epsilon_0\epsilon_r\mathbf{E} + \mathbf{P}, \ \ \mathbf{B} = \mu_0\mathbf{H}. \tag{1.2}$$

The parameters ϵ_0, and μ_0, are the permittivity, and permeability, respectively, of free space. The field vector $\mathbf{P}$ is called the macroscopic electric polarization, and the parameter ϵ_r is the relative permittivity of the dielectric. The constitutive relations (1.2) describe the response of a material to the electromagnetic fields.

In this abstract we concentrate our analyses on the single pole Debye polarization model, although the methods can be easily extended to Lorentz (see [1]) and multi-pole models.

1.1 Orientational Polarization: The Debye Model

A (single-pole) Debye model can be represented in (macroscopic) differential form as

$$\epsilon_0\epsilon_\infty\tau\frac{\partial \mathbf{E}}{\partial t} + \epsilon_0\epsilon_s\mathbf{E} = \tau\frac{\partial \mathbf{D}}{\partial t} + \mathbf{D}. \tag{1.3}$$

In equation (1.3), the parameter ϵ_s is the static relative permittivity. The presence of instantaneous polarization is accounted for by the coefficient $\epsilon_r = \epsilon_\infty$, the infinite frequency permittivity, in the electric flux equation in (1.2) and in the Debye model (1.3). The difference between these permittivities is commonly written $\epsilon_d := \epsilon_s - \epsilon_\infty$. The electric polarization driven by the electric field, less the part included in the instantaneous polarization, can be understood to be a decaying exponential with relaxation parameter τ.

2 Reduction to One Dimension

We consider the one dimensional case in which the electric field is assumed to be polarized to oscillate in the y direction and propagates in the z direction. Thus, we are only concerned with the scalar values $E(t,z)$, $D(t,z)$, and $B(t,z)$.

In this case Maxwell's equations (1.1) in the interior of the domain Ω become

$$\frac{\partial B}{\partial t} = \frac{\partial E}{\partial z}, \ \frac{\partial D}{\partial t} = \frac{1}{\mu_0}\frac{\partial B}{\partial z}. \tag{2.1}$$

3 $2M$ Order Spatial Approximations

In this section we describe the construction of higher order approximations to the first order derivative operator $\partial/\partial z$.

3.1 Staggered ℓ^2 Normed Spaces

We introduce the following staggered ℓ^2 normed spaces that will aid in obtaining the basic properties of the high order approximations. We define the *primary grid*, G_p, of $\mathbb{R}$, and the *dual grid*, G_d, of $\mathbb{R}$ both with space step size h to be

$$G_p = \{\ell h \mid \ell \in \mathbb{Z}\}, \tag{3.1}$$

$$G_d = \left\{\left(\ell + \frac{1}{2}\right) h \mid \ell \in \mathbb{Z}\right\}, \tag{3.2}$$

respectively. For any function v, we denote $v_\ell = v(\ell h)$ and $v_{\ell+\frac{1}{2}} = v((\ell+\frac{1}{2})h)$. We define staggered ℓ^2 normed spaces on G_p and G_d, respectively, as $V_0 = \{(v_\ell),\ \ell \in \mathbb{Z} |\ h\sum_{\ell\in\mathbb{Z}} |v_\ell|^2 \le \infty\}$, and $V_{\frac{1}{2}} = \left\{\left(v_{\ell+\frac{1}{2}}\right),\ \ell\in\mathbb{Z} |\ h\sum_{\ell\in\mathbb{Z}} |v_{\ell+\frac{1}{2}}|^2 \le \infty\right\}$, with scalar products $(\cdot,\cdot)_0$ and $(\cdot,\cdot)_{\frac{1}{2}}$ derived from the norms $||v||_0^2 = h\sum |v_\ell|^2$ and $||v||_{\frac{1}{2}}^2 = h\sum |v_{\ell+\frac{1}{2}}|^2$.

Next, we define the discrete operators $\mathcal{D}_{p,h}^{(2)} : V_0 \to V_{\frac{1}{2}}$ and $\tilde{\mathcal{D}}_{p,h}^{(2)} : V_{\frac{1}{2}} \to V_0$ by

$$\left(\mathcal{D}_{p,h}^{(2)} u\right)_{\ell+\frac{1}{2}} = \frac{u_{\ell+p} - u_{\ell-p+1}}{(2p-1)h}, \tag{3.3a}$$

$$\left(\tilde{\mathcal{D}}_{p,h}^{(2)} u\right)_{\ell} = \frac{u_{\ell+p-\frac{1}{2}} - u_{\ell-p+\frac{1}{2}}}{(2p-1)h}. \tag{3.3b}$$

These are second-order discrete approximations of the operator $\partial/\partial z$ computed with stepsize $(2p-1)h$.

3.2 Two Different Ways of Constructing Finite Difference Approximations

We construct finite difference approximations of order $2M$ of the first order operator $\partial/\partial z$, where $M \in \mathbb{N}$ is arbitrary. These approximations will be denoted as

$$\mathcal{D}_{1,h}^{(2M)} : V_0 \to V_{\frac{1}{2}}; \qquad \tilde{\mathcal{D}}_{1,h}^{(2M)} : V_{\frac{1}{2}} \to V_0. \tag{3.4}$$

The operators in (3.4) can be considered from two different points of view [2]

(V1) as linear combinations of second order approximations to $\partial/\partial z$ of the form (3.3) computed with different space steps, and

(V2) as a result of the truncation of an appropriate series expansion of the symbol of $\partial/\partial z$.

3.2.1 Series Expansion of the Symbol of $\partial/\partial z$

With respect to the second point of view, (V2), we can interpret the operators $\mathcal{D}_{1,h}^{(2M)}$ and $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ via their *symbols*. We define the symbol of a differential operator, as well as its finite difference approximation, via its application to harmonic plane waves [2]. Thus, if $v(z) = \mathrm{e}^{\mathrm{i}kz}$ then $\partial v/\partial z = \mathrm{i}kv(z)$, and

$$\mathcal{F}\left(\partial/\partial z\right) = \mathrm{i}k, \tag{3.5}$$

where $\mathcal{F}\left(\partial/\partial z\right)$ denotes the symbol of the differential operator $\partial/\partial z$. We can show that the symbol of the finite difference operator $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ (or $\mathcal{D}_{1,h}^{(2M)}$) can be written as

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2\mathrm{i}}{h}\sum_{j=1}^{M} \frac{\lambda_{2j-1}^{2M}}{2j-1}\sin(kh(2j-1)/2), \tag{3.6}$$

where for $1 \le p \le M$,

$$\lambda_{2p-1}^{2M} = \frac{2(-1)^{p-1}[(2M-1)!!]^2}{(2M+2p-2)!!(2M-2p)!!(2p-1)}, \tag{3.7}$$

and the double factorial is defined as

$$n!! = \begin{cases} n\cdot(n-2)\cdot(n-4)\ldots 5\cdot 3\cdot 1 & n>0,\ \text{odd} \\ n\cdot(n-2)\cdot(n-4)\ldots 6\cdot 4\cdot 2 & n>0,\ \text{even} \\ 1, & n=-1,0. \end{cases}$$

We now introduce the following alternative formulation of the symbol of the operator $\tilde{\mathcal{D}}_{1,h}^{(2M)}$.

Theorem 1 ([1]) *The symbol of the operator $\tilde{\mathcal{D}}_{1,h}^{(2M)}$ can be rewritten in the form*

$$\mathcal{F}\left(\tilde{\mathcal{D}}_{1,h}^{(2M)}\right) = \frac{2\mathrm{i}}{h}\sum_{p=1}^{M} \gamma_{2p-1}\sin^{2p-1}(kh/2), \tag{3.8}$$

where the coefficients γ_{2p-1} are strictly positive, independent of M, and are given by the explicit formula

$$\gamma_{2p-1} = \frac{[(2p-3)!!]^2}{(2p-1)!}. \tag{3.9}$$

The coefficients γ_{2p-1}, defined in (3.9), *are the coefficients in the Taylor expansion of the function* $\sin^{-1} x$ *around zero.*

Lemma 1 *The series $\sum_{p=1}^{\infty} \gamma_{2p-1}$ is convergent and its sum is $\pi/2$.*

In Table 1 we provide the coefficients γ_{2p-1} for various values of p.

Table 1: The first four coefficients γ_{2p-1}

γ_1	γ_3	γ_5	γ_7
1	$\frac{1}{6}$	$\frac{3}{40}$	$\frac{5}{112}$

4 High Order Numerical Methods for Debye Dispersive Media

In this section we construct a family of finite difference schemes for Maxwell's equations in Debye dispersive media in 1D. These schemes are based on the discrete higher order ($2M,\ M \in \mathbb{N}$) approximations to the first order operator that were constructed in Section 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 Yee scheme, or FDTD scheme, for Maxwell's equations to dispersive media.

The $(2, 2M)$ discretized schemes for Maxwell's equations (2.1) in 1D are

$$\frac{B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n-\frac{1}{2}}_{j+\frac{1}{2}}}{\Delta t} = \sum_{p=1}^{M} \lambda^{2M}_{2p-1} \left(\mathcal{D}^{(2)}_{p,\Delta z} E\right)_{j+\frac{1}{2}}, \quad (4.1a)$$

$$\frac{D^{n+1}_{j} - D^{n}_{j}}{\Delta t} = \frac{1}{\mu_0} \sum_{p=1}^{M} \lambda^{2M}_{2p-1} \left(\tilde{\mathcal{D}}^{(2)}_{p,\Delta z} B\right)_{j}, \quad (4.1b)$$

where, λ^{2M}_{2p-1} is defined in (3.7), and the discrete operators $\mathcal{D}^{(2)}_{p,\Delta z}$ and $\tilde{\mathcal{D}}^{(2)}_{p,\Delta z}$ are defined in (3.3) with $h = \Delta z$.

4.1 $(2, 2M)$ Numerical Methods for Debye Media

For a Debye media we add the discretized (in time) version of the equation (1.3) given as

$$\epsilon_0\epsilon_\infty\tau \frac{E^{n+1}_j - E^n_j}{\Delta t} + \epsilon_0\epsilon_s \frac{E^{n+1}_j + E^n_j}{2} = \tau \frac{D^{n+1}_j - D^n_j}{\Delta t} + \frac{D^{n+1}_j + D^n_j}{2}, \quad (4.1c)$$

to the system defined in (4.1a) and (4.1b).

5 von Neumann Stability Analysis

We look for plane wave solutions of (a scaled version of) (2.1) with (1.3) as numerically evaluated at the discrete space-time point (t^n, z_j), or $(t^{n+1/2}, z_{j+1/2})$. We assume a spatial dependence of the form, e.g.,

$$B^{n+\frac{1}{2}}_{j+\frac{1}{2}} = \hat{B}^{n+\frac{1}{2}}(k)\mathrm{e}^{\mathrm{i}kz_{j+\frac{1}{2}}};\ E^n_j = \hat{E}^n(k)\mathrm{e}^{\mathrm{i}kz_j} \quad (5.1)$$

in the field quantities, with k defined to be the wavenumber. Define the vector $\mathbf{U}^n := [c_\infty \hat{B}^{n-\frac{1}{2}}, \hat{E}^n, \frac{1}{\epsilon_0\epsilon_\infty}\hat{D}^n]^T$, where $c_\infty^2 := 1/(\epsilon_0\mu_0\epsilon_\infty)$. Substituting the forms (5.1) into the higher order schemes (4.1), and canceling out common terms we obtain the system $\mathbf{U}^{n+1} = \mathcal{A}\mathbf{U}^n$. The characteristic polynomial of $\mathcal{A}$ is given by

$$P^{\mathrm{D}}_{(2,2M)}(\zeta) = \zeta^3 + \left(\frac{q\epsilon_\infty(2+h_\tau) - (6\epsilon_\infty + h_\tau\epsilon_s)}{2\epsilon_\infty + h_\tau\epsilon_s}\right)\zeta^2 + \left(\frac{q\epsilon_\infty(h_\tau - 2) + (6\epsilon_\infty - h_\tau\epsilon_s)}{2\epsilon_\infty + h_\tau\epsilon_s}\right)\zeta - \left(\frac{2\epsilon_\infty - h_\tau\epsilon_s}{2\epsilon_\infty + h_\tau\epsilon_s}\right)$$

where $h_\tau := \Delta t/\tau$, $\epsilon_q := \epsilon_s/\epsilon_\infty$, $q := |\sigma|^2$ and

$$\sigma := -\eta\Delta z \mathcal{F}\left(\tilde{\mathcal{D}}^{(2M)}_{1,\Delta z}\right). \quad (5.2)$$

The parameter η is the Courant (stability) number $\eta := (c_\infty \Delta t)/\Delta z$, where c_∞ is the maximum speed of light in the Debye medium.

Theorem 2 ([1]) *A necessary and sufficient stability condition for the $(2, 2M)$ scheme in (4.1) is that*

$$4\eta^2 \left(\sum_{p=1}^{M} \gamma_{2p-1} \sin^{2p-1}\left(\frac{k\Delta z}{2}\right)\right)^2 < 4,\ \forall k, \quad (5.3)$$

which implies that $\eta\left(\sum_{p=1}^{M} \gamma_{2p-1}\right) < 1$, or that

$$\Delta t < \frac{\Delta z}{\left(\sum_{p=1}^{M} \frac{[(2p-3)!!]^2}{(2p-1)!}\right) \mathrm{c}_\infty}. \quad (5.4)$$

In the limiting case (as $M \to \infty$), we may evaluate the infinite series using Lemma 1. Therefore,

$$M = \infty,\ \eta\left(\frac{\pi}{2}\right) < 1 \Longleftrightarrow \Delta t < \frac{2\Delta z}{\pi\ \mathrm{c}_\infty}. \quad (5.5)$$

The positivity of the coefficients γ_{2p-1} gives that the constraint on Δt in (5.5) is a lower bound on all constraints for any $M \in \mathbb{N}$. Therefore this constraint guarantees stability for all orders.

6 Dispersion Analysis

We assume plane wave solutions of the form $e^{i(k^{\mathrm{D}}_{\mathrm{FD},M} j\Delta z - \omega n \Delta t)}$, where $k^{\mathrm{D}}_{\mathrm{FD},M}$ represents the numerical wave number. By considering plane wave solutions for all the discrete variables in the $(2,2M)$ finite difference schemes for Debye media given in (4.1), we can derive the numerical dispersion relation of this scheme. First, we define the following quantity which relates the order of the method to the resulting numerical wavenumber $k^{\mathrm{D}}_{\mathrm{FD},M}$,

$$K^{\mathrm{D}}_{\mathrm{FD},M}(\omega) := \frac{2}{\Delta z}\sum_{p=1}^{M}\gamma_{2p-1}\sin^{2p-1}\left(\frac{k^{\mathrm{D}}_{\mathrm{FD},M}(\omega)\Delta z}{2}\right),$$

where the coefficients γ_{2p-1} are those defined in Theorem 1. Thus, the numerical dispersion relations of the $(2,2M)$ schemes for the Debye model, which implicitly give $k^{\mathrm{D}}_{\mathrm{FD},M}$ as a function of discretization parameters and ω, can be succinctly written as

$$K^{\mathrm{D}}_{\mathrm{FD},M}(\omega) = \frac{\omega_\Delta}{c}\sqrt{\epsilon^{\mathrm{D}}_{r,\mathrm{FD}}}; \quad \epsilon^{\mathrm{D}}_{r,\mathrm{FD}} := \frac{\epsilon_{s,\Delta}\lambda_\Delta - i\omega_\Delta\epsilon_{\infty,\Delta}}{\lambda_\Delta - i\omega_\Delta},$$

where the parameters $\epsilon_{s,\Delta} := \epsilon_s$; $\epsilon_{\infty,\Delta} := \epsilon_\infty$; $\lambda_\Delta := \lambda\cos(\omega\Delta t/2)$, 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 $\omega_\Delta := \omega\dfrac{\sin(\omega\Delta t/2)}{\omega\Delta t/2}$.

We define the phase error Φ to be

$$\Phi = \left|\frac{k_{\mathrm{EX}} - k^{\mathrm{D}}_{\mathrm{FD},M}}{k_{\mathrm{EX}}}\right|, \qquad (6.1)$$

where the numerical wave number $k^{\mathrm{D}}_{\mathrm{FD},M}$ is implicitly determined by the corresponding dispersion relation and k_{EX} is the exact wave number for the Debye model. We wish to examine the phase error as a function of $\omega\Delta t$ in the range $[0,\pi]$.

In Figure 1 we depict the phase error Φ defined in (6.1), versus $\omega\Delta t$, for (spatial) orders $2M = 2,4,6,8$ and the limiting $(M=\infty)$ case, with the parameters: $\epsilon_\infty = 1$; $\epsilon_s = 78.2$; $\tau = 8.1\times 10^{-12}$ sec. These are appropriate constants for modeling water and are representative of a large class of Debye type materials. In [1] we provide comparisons of different order methods by considering these dispersion plots for different values of h_τ and η.

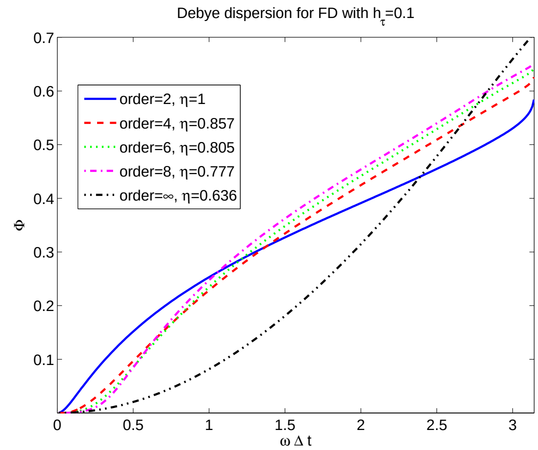

Figure 1: Phase error ϕ using $h_\tau = 0.1$ with η set to the maximum stable value for the order.

7 Conclusions

For each order of scheme we have given a necessary and sufficient stability condition which is explicitly dependent on the material parameters and the order of the method. Additionally, we have found a bound for stability for all orders by computing the limiting (infinite order) case. Further, 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.

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References

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