Stability of FD–TD schemes for Maxwell–Debye and Maxwell–Lorentz equations.

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Abstract

The stability of five finite difference–time domain (FD–TD) schemes coupling Maxwell equations to Debye or Lorentz models have been analyzed in [1], where numerical evidence for specific media have been used. We use von Neumann analysis to give necessary and sufficient stability conditions for these schemes for any medium, in accordance with the partial results of [1].

Keywords : Stability analysis, Maxwell–Debye, Maxwell–Lorentz.

1 Introduction

To describe the propagation of an electromagnetic wave through a dispersive medium some extensions to Maxwell equations are used. They involve time differential equations which accounts for the constitutive laws of the material that link the displacement $\mathbf{D}$ to the electric field $\mathbf{E}$ or equivalently the polarization $\mathbf{P}$ to $\mathbf{E}$. We focus on two of these models (Debye and Lorentz models) which are addressed in [1] in view of specific applications to the interaction of an electromagnetic wave with a human body. In contrast we treat any medium which is described by these models. We only consider the stability analysis of numerical schemes whereas [1] also treated phase error issues.

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1.1 Maxwell–Debye and Maxwell–Lorentz models

In our context (no magnetization) the Maxwell equations read

$$\begin{aligned} \text{(Faraday)} \quad \partial_t \mathbf{B}(t,\mathbf{x}) &= -\operatorname{curl} \mathbf{E}(t,\mathbf{x}), \\ \text{(Ampère)} \quad \partial_t \mathbf{D}(t,\mathbf{x}) &= \frac{1}{\mu_0} \operatorname{curl} \mathbf{B}(t,\mathbf{x}), \end{aligned} \tag{1}$$

where $\mathbf{x} \in \mathbb{R}^N$ together with a linear constitutive law

$$\mathbf{D}(t,\mathbf{x}) = \varepsilon_0 \varepsilon_\infty \mathbf{E}(t,\mathbf{x}) + \varepsilon_0 \int_{-\infty}^{t} \mathbf{E}(t-\tau,\mathbf{x}) \chi(\tau) d\tau, \tag{2}$$

where ε_∞ is the relative infinite frequency permittivity and χ is the linear susceptibility. The discretization of the integral expression (2) leads to recursive schemes (see e.g. [2], [3]). However, differentiating Eq. (2) leads to a time differential equation for $\mathbf{D}$ which depends on the specific form of χ. For a Debye medium

$$t_{\mathrm{r}} \partial_t \mathbf{D} + \mathbf{D} = t_{\mathrm{r}} \varepsilon_0 \varepsilon_\infty \partial_t \mathbf{E} + \varepsilon_0 \varepsilon_{\mathrm{s}} \mathbf{E}, \tag{3}$$

where $t_{\mathrm{r}} > 0$ is the relaxation time and $\varepsilon_{\mathrm{s}} \geq \varepsilon_\infty$ is the relative static permittivity. Defining the polarization by $\mathbf{P}(t,\mathbf{x}) = \mathbf{D}(t,\mathbf{x}) - \varepsilon_0 \varepsilon_\infty \mathbf{E}(t,\mathbf{x})$, an equivalent form is

$$t_{\mathrm{r}} \partial_t \mathbf{P} + \mathbf{P} = \varepsilon_0 (\varepsilon_{\mathrm{s}} - \varepsilon_\infty) \mathbf{E}. \tag{4}$$

For a Lorentz medium with one resonant frequency ω_1, we likewise have

$$\partial_t^2 \mathbf{D} + \nu \partial_t \mathbf{D} + \omega_1^2 \mathbf{D} = \varepsilon_0 \varepsilon_\infty \partial_t^2 \mathbf{E} + \varepsilon_0 \varepsilon_\infty \nu \partial_t \mathbf{E} + \varepsilon_0 \varepsilon_{\mathrm{s}} \omega_1^2 \mathbf{E}, \tag{5}$$

where $\nu \geq 0$ is a damping coefficient, and

$$\partial_t^2 \mathbf{P} + \nu \partial_t \mathbf{P} + \omega_1^2 \mathbf{P} = \varepsilon_0 (\varepsilon_{\mathrm{s}} - \varepsilon_\infty) \omega_1^2 \mathbf{E}. \tag{6}$$

If we denote by $\mathbf{J}$ the time derivative of $\mathbf{P}$, system (1) can be cast as

$$\begin{aligned} \partial_t \mathbf{B}(t,\mathbf{x}) &= -\operatorname{curl} \mathbf{E}(t,\mathbf{x}), \\ \varepsilon_0 \varepsilon_\infty \partial_t \mathbf{E}(t,\mathbf{x}) &= \frac{1}{\mu_0} \operatorname{curl} \mathbf{B}(t,\mathbf{x}) - \mathbf{J}(t,\mathbf{x}). \end{aligned} \tag{7}$$

1.2 Numerical schemes

A classical and very efficient way to compute the Maxwell equations is the Yee scheme [4]. We restrict our study to existing Yee based schemes. Other methods may be found in the literature in the context of Maxwell-Debye and Maxwell-Lorentz equations: see e.g. [5] for pseudo-spectral schemes or [6] for finite element–time domain (FE–TD) schemes.

The Yee scheme consists in discretizing $\mathbf{E}$ and $\mathbf{B}$ on staggered grids in space and time. This allows to use only centered discrete differential operators. We denote by h the space step (supposed here to be the same in all directions in the case of multi-dimensional equations) and by k the time step. In space dimension 1, we only consider the dependence in the space variable z and classically two polarizations for the field may be decoupled. For example, the transverse electric polarization only involves $E \equiv E_x$ and $B \equiv B_y$. The discretized variables are $E_j^n \simeq E(nk, jh)$ (and similar notations for $D \equiv D_x$) and $B_{j+\frac{1}{2}}^{n+\frac{1}{2}} \simeq B((n+\frac{1}{2})k, (j+\frac{1}{2})h)$, and the Yee scheme for system (1) reads

$$\begin{aligned} \frac{1}{k}(B_{j+\frac{1}{2}}^{n+\frac{1}{2}} - B_{j+\frac{1}{2}}^{n-\frac{1}{2}}) &= -\frac{1}{h}(E_{j+1}^n - E_j^n), \\ \frac{1}{k}(D_j^{n+1} - D_j^n) &= -\frac{1}{\mu_0 h}(B_{j+\frac{1}{2}}^{n+\frac{1}{2}} - B_{j-\frac{1}{2}}^{n+\frac{1}{2}}). \end{aligned} \tag{8}$$

Similarly the Yee scheme for system (7) reads

$$\begin{aligned} \frac{1}{k}(B_{j+\frac{1}{2}}^{n+\frac{1}{2}} - B_{j+\frac{1}{2}}^{n-\frac{1}{2}}) &= -\frac{1}{h}(E_{j+1}^n - E_j^n), \\ \frac{\varepsilon_0\varepsilon_\infty}{k}(E_j^{n+1} - E_j^n) &= -\frac{1}{\mu_0 h}(B_{j+\frac{1}{2}}^{n+\frac{1}{2}} - B_{j-\frac{1}{2}}^{n+\frac{1}{2}}) - J_j^{n+\frac{1}{2}}. \end{aligned} \tag{9}$$

Usual Maxwell equations consist in taking $J_j^{n+\frac{1}{2}} \equiv 0$ in Eq. (9) or equivalently $D_j^n = \varepsilon_0\varepsilon_\infty E_j^n$ in Eq. (8) and leads to a stable second order scheme under a Courant–Friedrichs–Lewy (CFL) stability condition. Namely, if $c_\infty = 1/\sqrt{\varepsilon_0\varepsilon_\infty\mu_0}$ denotes the infinite frequency light speed, the CFL condition reads $c_\infty k \leq h$ if the space dimension is $N = 1$ and $c_\infty k \leq h/\sqrt{2}$ for $N = 2$ or 3.

In contrast to the recursive schemes, we are interested in direct integration schemes which are based on the finite difference–time domain (FD–TD) discretization of Eqs (3) to (6) (see [7], [8], [9]).

1.3 Outline

The von Neumann stability analysis is recalled in Sect. 2. We also describe the sketch of our proofs which is common for all the schemes. In Section 3 two one dimensional direct integration schemes for Debye media are presented and analyzed, pointing carefully out the physical properties needed to ensure stability and the specific cases which have to be handled separately. Numerical applications to physical media are also given. The same point of view is carried out for Lorentz media in Section 4. Two-dimensional results are given in Section 5.

2 Principles of the von Neumann analysis

The von Neumann analysis allows to localize roots of certain classes of polynomials, which proves to be crucial here. We recall the main principles of this technique. Details and proofs of theorems may be found in [10].

2.1 Schur and von Neumann polynomials

We define two families of polynomials: Schur polynomials and simple von Neumann polynomials.

Definition 1 *A polynomial is a Schur polynomial if all its roots, r, satisfy $|r| < 1$.*

Definition 2 *A polynomial is a simple von Neumann polynomial if all its roots, r, lie on the unit disk ($|r| \leq 1$) and its roots on the unit circle are simple roots.*

If a polynomial is of high degree or has sophisticated coefficients, it may be difficult to locate its roots. However, there is a way to split this difficult problem into many simpler ones. For this aim, we construct a sequence of polynomials of decreasing degree. Let ϕ be written as

$$\phi(z) = c_0 + c_1 z + \cdots + c_p z^p,$$

where c_0, c_1 ..., $c_p \in \mathbb{C}$ and $c_p \neq 0$. We define its conjugate polynomial ϕ^* by

$$\phi^*(z) = c_p^* + c_{p-1}^* z + \cdots + c_0^* z^p.$$

Given a polynomial ϕ_0, we may define a sequence of polynomials

$$\phi_{m+1}(z) = \frac{\phi_m^*(0)\phi_m(z) - \phi_m(0)\phi_m^*(z)}{z}.$$

It is clear that $\deg\phi_{m+1} < \deg\phi_m$, if $\phi_m \not\equiv 0$. Besides, we have the two following theorems.

Theorem 1 *A polynomial ϕ_m is a Schur polynomial of exact degree d if and only if ϕ_{m+1} is a Schur polynomial of exact degree $d-1$ and $|\phi_m(0)| \leq |\phi_m^*(0)|$.*

Theorem 2 *A polynomial ϕ_m is a simple von Neumann polynomial if and only if*

- *ϕ_{m+1} is a simple von Neumann polynomial and $|\phi_m(0)| \leq |\phi_m^*(0)|$,*

or

- *ϕ_{m+1} is identically zero and ϕ_m' is a Schur polynomial.*

The main ingredient in the proof of both theorems is the Rouché theorem (see [10]). To analyze ϕ_0, at each step m, conditions should be checked (leading coefficient is non-zero, $|\phi_m(0)| \leq |\phi_m^*(0)|, \ldots$) until a definitive negative answer arises or the degree is 1.

2.2 Stability analysis

The models we deal with are linear models. They may therefore be analyzed in the frequency domain. Thus we assume that the scheme handles a variable $U_{\mathbf{j}}^n$ with spatial dependence

$$U_{\mathbf{j}}^n = U^n \exp(i\boldsymbol{\xi} \cdot \mathbf{j}),$$

where $\boldsymbol{\xi}$ and $\mathbf{j} \in \mathbb{R}^N$, $N = 1, 2, 3$. The amplification matrix G is the matrix such that $U^{n+1} = GU^n$. We assume that G does not depend on time or on h and k separately but only on the ratio h/k. Let ϕ_0 be the characteristic polynomial of G, then we have a sufficient stability condition.

Theorem 3 *A sufficient stability condition is that ϕ_0 be a simple von Neumann polynomial.*

This condition is not necessary. A scheme is stable if and only if the sequence $(U^n)_{n\in\mathbb{N}}$ is bounded. Since we assume that G does not depend on time, $U^n = G^n U^0$ and stability is also the boundedness of $(G^n)_{n\in\mathbb{N}}$. If the eigenvalues of G, i.e. the roots r of ϕ_0, lie inside the unit circle ($|r| < 1$), then $\lim_{n\to\infty} G^n = 0$ and the sequence is bounded. If any root lies outside the unit circle then G^n grows exponentially and the scheme is unstable. The intermediate case when some roots may be on the unit circle (and the others inside) may lead to different situations. The good case is for example given when G

is the identity. Then $U^n = U^0$ and the scheme is clearly stable. However there are other examples of matrices with multiple roots on the unit circle that lead either to bounded or unbounded sequences $(G^n)_{n\in\mathbb{N}}$. We will call this property G^n-boundedness in the sequel. It is clearly a property of the amplification matrix and not of its characteristic polynomial. If the minimal stable subspaces associated to the multiple root are one-dimensional then G^n is bounded (identity example). If the minimal stable subspaces are multidimensional then G^n grows linearly. Such cases (which occur for our schemes) should therefore be handled specifically.

2.3 Sketch of proofs

In the next sections, we will not give the proofs, but only list in a table the arguments used for each situation. We describe here the general plan and give names to specific final arguments used. The detailed proofs may be found in [11] for space dimensions 1 and 2. The three dimensional case is much more tedious and is work in progress.

Usually the system is given in a implicit form. The first step consists in writing it in an explicit form. This yields the amplification matrix G. Then we compute its characteristic polynomial ϕ_0. In order to perform a von Neumann analysis, we compute the series (ϕ_m). In the general case, under the assumption that the stability condition cannot be better than Maxwell's, we can apply either Theorem 1 (*Theorem 1* argument) or Theorem 2 (*Theorem 2* argument), check estimates at each level until ϕ_m is a one degree polynomial. Special cases arise when $\varepsilon_{\rm s} = \varepsilon_\infty$, $\sin(\xi/2) = 0$ or ± 1, and sometimes for limit values of physical coefficients. In these cases, different points of view have to be considered:

- Theorem 2 has to be used instead of Theorem 1,
- Some eigenvalues lie on the unit circle (mostly ± 1 or $\pm i$) and are simple, it is then sufficient to study only the other eigenvalues (*sub-polynomial* argument) and we conclude to a simple von Neumann polynomial and stability,
- Some eigenvalues lie on the unit circle and are not simple, and besides the study of the other eigenvalues (to prove that the polynomial is a von Neumann one), we have to find out if the associated minimal stable subspaces are one- (stable case) or multidimensional (unstable case). This may be checked directly on the form of matrix G (*G form*

argument), or necessitates the computation of eigenvectors (*eigenvectors* argument). If only one eigendirection is found for a multiple eigenvalue, the minimal subspace is necessarily multidimensional.

3 Debye media

We address two discretizations of Maxwell–Debye equations. The first one uses a $(\mathbf{B}, \mathbf{E}, \mathbf{D})$ setting for the equations and the second a $(\mathbf{B}, \mathbf{E}, \mathbf{P}, \mathbf{J})$ formulation.

3.1 Debye–Joseph et al. model

In [8], Joseph et al. close System (8) by a discretization for Eq. (3), namely

$$\varepsilon_0 \varepsilon_\infty t_\mathrm{r} \frac{E_j^{n+1} - E_j^n}{k} + \varepsilon_0 \varepsilon_\mathrm{s} \frac{E_j^{n+1} + E_j^n}{2} = t_\mathrm{r} \frac{D_j^{n+1} - D_j^n}{k} + \frac{D_j^{n+1} + D_j^n}{2}. \tag{10}$$

System (8)–(10) may be cast in an explicit form which handles the variable

$$U_j^n = {}^t(c_\infty B_{j+\frac{1}{2}}^{n-\frac{1}{2}}, E_j^n, D_j^n / \varepsilon_0 \varepsilon_\infty)$$

and the amplification matrix G reads

$$\begin{pmatrix} 1 & -\lambda(e^{i\xi} - 1) & 0 \\ -\frac{(1+\delta)\lambda(1-e^{-i\xi})}{1+\delta\varepsilon'_\mathrm{s}} & \frac{(1-\delta\varepsilon'_\mathrm{s}) + (1+\delta)\lambda^2(e^{i\xi}-2+e^{-i\xi})}{1+\delta\varepsilon'_\mathrm{s}} & \frac{2\delta}{1+\delta\varepsilon'_\mathrm{s}} \\ -\lambda(1 - e^{-i\xi}) & \lambda^2(e^{i\xi} - 2 + e^{-i\xi}) & 1 \end{pmatrix}$$

where $\lambda = c_\infty k/h$ is the CFL constant, $\delta = k/2t_\mathrm{r} > 0$ is the normalized time step and $\varepsilon'_\mathrm{s} = \varepsilon_\mathrm{s}/\varepsilon_\infty \geq 1$ denotes the normalized static permittivity. Moreover we define

$$q = -\lambda^2(e^{i\xi} - 2 + e^{-i\xi}) = 4\lambda^2 \sin^2(\xi/2).$$

The characteristic polynomial is proportional to

$$\begin{aligned} \phi_0(Z) \;=\; & [1 + \delta\varepsilon'_\mathrm{s})]Z^3 - [3 + \delta\varepsilon'_\mathrm{s} - (1+\delta)q]Z^2 \\ & + [3 - \delta\varepsilon'_\mathrm{s} - (1-\delta)q]Z - [1 - \delta\varepsilon'_\mathrm{s}]. \end{aligned}$$

The proofs are summed up in Table 1 and we deduce that the stability condition is $q \leq 4$ if $\varepsilon_\mathrm{s} > \varepsilon_\infty$ and $q < 4$ if $\varepsilon_\mathrm{s} = \varepsilon_\infty$.

q	ε_{s}	argument	result
$]0,4[$	$>\varepsilon_\infty$	Theorem 1	stable
$]0,4[$	$=\varepsilon_\infty$	Theorem 2	stable
0	$\geq\varepsilon_\infty$	G form	stable
4	$>\varepsilon_\infty$	Theorem 2	stable
4	$=\varepsilon_\infty$	eigenvectors	unstable

Table 1: Proof arguments and results for the Debye–Joseph et al. model.

3.2 Debye–Young model

In [9], Young closes System (9) by two discretizations for Eq. (4), namely

$$t_{\mathrm{r}}\frac{P_j^{n+\frac{1}{2}}-P_j^{n-\frac{1}{2}}}{k}=-\frac{P_j^{n+\frac{1}{2}}+P_j^{n-\frac{1}{2}}}{2}+\varepsilon_0(\varepsilon_{\mathrm{s}}-\varepsilon_\infty)E_j^n, \tag{11}$$

$$t_{\mathrm{r}}J_j^{n+\frac{1}{2}}=-P_j^{n+\frac{1}{2}}+\varepsilon_0(\varepsilon_{\mathrm{s}}-\varepsilon_\infty)\frac{E_j^{n+1}+E_j^n}{2}. \tag{12}$$

Although $J_j^{n+\frac{1}{2}}$ is used for the computations, this not a genuine variable for System (9)–(11)–(12) which handles the variable

$$U_j^n={}^t(c_\infty B_{j+\frac{1}{2}}^{n-\frac{1}{2}},E_j^n,P_j^{n-\frac{1}{2}}/\varepsilon_0\varepsilon_\infty)$$

and the amplification matrix G reads

$$\begin{pmatrix} 1 & -\lambda(e^{i\xi}-1) & 0 \\ -\frac{\lambda(1-e^{-i\xi})}{1+\delta\alpha} & \frac{1+\delta-\delta\alpha+3\delta^2\alpha-(1+\delta)q}{(1+\delta)(1+\delta\alpha)} & \frac{1-\delta}{1+\delta}\frac{2\delta}{1+\delta\alpha} \\ 0 & \frac{2\delta\alpha}{1+\delta} & \frac{1-\delta}{1+\delta} \end{pmatrix}$$

with the same notation as above and $\alpha=\varepsilon_{\mathrm{s}}'-1\geq 0$.

The characteristic polynomial is proportional to

$$\begin{aligned}\phi_0(Z) &= [(1+\delta\alpha)(1+\delta)]Z^3-[3+\delta+\delta\alpha+3\delta^2\alpha-(1+\delta)q]Z^2 \\ &\quad +[3-\delta-\delta\alpha+3\delta^2\alpha-(1-\delta)q]Z-[(1-\delta\alpha)(1-\delta)].\end{aligned}$$

Again, the proofs are summed up in Table 2.

The stability condition is therefore $q\leq 4$ and $\delta\leq 1$ if $\varepsilon_{\mathrm{s}}>\varepsilon_\infty$ and $q<4$ if $\varepsilon_{\mathrm{s}}=\varepsilon_\infty$.

q	ε_{s}	δ	argument	result
$]0,4]$	$> \varepsilon_\infty$	$]0,1[$	Theorem 1	stable
$]0,4[$	$= \varepsilon_\infty$	> 0	Theorem 2	stable
0	$\geq \varepsilon_\infty$	> 0	G form	stable
$]0,4]$	$> \varepsilon_\infty$	1	sub-polynomial	stable
4	$= \varepsilon_\infty$	> 0	eigenvectors	unstable

Table 2: Proof arguments and results for the Debye–Young model.

3.3 Conclusion for one-dimensional Debye schemes

If $\varepsilon_{\mathrm{s}} > \varepsilon_\infty$, the pure CFL condition $q \leq 4$ is the same for both models. It is exactly the condition for Maxwell equations. However Young model necessitates another condition, $\delta \leq 1$, which corresponds to a sufficient discretization of Debye equation (4). Even if we are interested here in stability properties, such conditions are to be taken to ensure equations to be correctly taken into account. Results are given in physical variables in Table 3.

Scheme		dimension 1
	$\varepsilon_{\mathrm{s}} > \varepsilon_\infty$	
Joseph et al.	$q \leq 4$	$k \leq \frac{h}{c_\infty}$
Young	$q \leq 4,\ \delta \leq 1$	$k \leq \min(\frac{h}{c_\infty}, 2t_{\mathrm{r}})$
	$\varepsilon_{\mathrm{s}} = \varepsilon_\infty$	
Joseph et al.	$q < 4$	$k < \frac{h}{c_\infty}$
Young	$q < 4$	$k < \frac{h}{c_\infty}$

Table 3: Stability of Debye models for $\varepsilon_{\mathrm{s}} > \varepsilon_\infty$ and $\varepsilon_{\mathrm{s}} = \varepsilon_\infty$.

To compare conditions on q and δ, let us consider a simple physical case. We assume that a matter with $\varepsilon_\infty = 1$ (and thus $c_\infty \simeq 3\,10^8\,\mathrm{m\,s^{-1}}$) is lighted by an optical wave of say wavelength $1\,\mu\mathrm{m}$. The space step h has to be smaller than this wavelength, and therefore $q < 4$ reads at least $k < \frac{1}{3}\,10^{-14}\,\mathrm{s}$. In a Debye medium, relaxation times t_{r} are of the order of a picosecond (or even a nanosecond) which is many decades larger than the previous bound. The estimate $q < 4$ is thus predominant and both models present the same advantages. Only the value of ε_∞ yields the CFL condition. A typical example is water for which $\varepsilon_\infty = 1.8$, $\varepsilon_{\mathrm{s}} = 81.0$ and $t_{\mathrm{r}} = 9.4\,10^{-12}\,\mathrm{s}$ [3]. Condition $k \leq 2t_{\mathrm{r}}$ comes to $k \leq 1.88\,10^{-11}\,\mathrm{s}$. Condition

$q \leq 4$ yields a similar condition if $h = 4.2\,10^{-3}$ m. This is of course much larger than any reasonable space step for Maxwell equations and optical waves. The stability condition for water is $q < 4$ for both schemes. A quite different material is for example the 0.25-dB loaded foam given in [12] for which $\varepsilon_\infty = 1.01$, $\varepsilon_{\rm s} = 1.16$ and $t_{\rm r} = 6.497\,10^{-10}$ s. Condition $k \leq 2t_{\rm r}$ comes to $k \leq 1.3\,10^{-9}$ s and $q \leq 4$ yields a similar condition if $h = 3.9\,10^{-1}$ m. Once more, the stability condition for water is $q < 4$ for both schemes.

In conclusion for current material the stability condition is the same for Maxwell–Debye equations as for the usual Yee scheme. The result announced in [1] was $q \leq 4$ for Joseph et al. scheme and for water, which is consistent with our result.

4 Lorentz media

Three discretizations of Maxwell–Lorentz equations are now addressed. The first one uses a $(\mathbf{B}, \mathbf{E}, \mathbf{D})$ setting and the two others a $(\mathbf{B}, \mathbf{E}, \mathbf{P}, \mathbf{J})$ formulation, but differ from the time-discretization of $\mathbf{J}$.

Each of these models reads the same in the harmonic ($\nu = 0$) or anharmonic ($\nu > 0$) cases. However the analysis will differ greatly since $\phi_1 \equiv 0$ for all the schemes in the harmonic cases.

4.1 Lorentz–Joseph et al. model

In [8], system (8) is closed by a discretization for Eq. (3), namely

$$\begin{aligned}\varepsilon_0\varepsilon_\infty \frac{E_j^{n+1} - 2E_j^n + E_j^{n-1}}{k^2} + \nu\varepsilon_0\varepsilon_\infty \frac{E_j^{n+1} - E_j^{n-1}}{2k} + \varepsilon_0\varepsilon_{\rm s}\omega_1^2 \frac{E_j^{n+1} + E_j^{n-1}}{2} \\ = \frac{D_j^{n+1} - 2D_j^n + D_j^{n-1}}{k^2} + \nu \frac{D_j^{n+1} - D_j^{n-1}}{2k} + \omega_1^2 \frac{D_j^{n+1} + D_j^{n-1}}{2}\end{aligned} \tag{13}$$

The explicit version of system (8)–(13) does not use explicitly the value of D_j^{n-1} and therefore this system handles the variable

$$U_j^n = {}^t(c_\infty B_{j+\frac{1}{2}}^{n-\frac{1}{2}}, E_j^n, E_j^{n-1}, D_j^n/\varepsilon_0\varepsilon_\infty).$$

The amplification matrix G reads

$$\begin{pmatrix} 1 & -\lambda(e^{i\xi} - 1) & 0 & 0 \\ -\frac{2\delta\lambda(1-e^{-i\xi})}{1+\delta+\omega\varepsilon'_{\rm s}} & \frac{2-q(1+\delta+\omega)}{1+\delta+\omega\varepsilon'_{\rm s}} & \frac{1-\delta+\omega\varepsilon'_{\rm s}}{1+\delta+\omega\varepsilon'_{\rm s}} & \frac{2\omega}{1+\delta+\omega\varepsilon'_{\rm s}} \\ 0 & 1 & 0 & 0 \\ -\lambda(1 - e^{-i\xi}) & -q & 0 & 1 \end{pmatrix}$$

where $\delta = \nu k/2 \geq 0$ is the new normalized time step, and $\omega = \omega_1^2 k^2/2 > 0$ denotes the normalized squared frequency. The other notations used for the Debye model remain valid.

The characteristic polynomial is proportional to

$$\begin{aligned}\phi_0(Z) &= [1+\delta+\omega\varepsilon_s']Z^4 - [4+2\delta+2\omega\varepsilon_s' - (1+\delta+\omega)q]Z^3 \\ &+[6+2\omega\varepsilon_s' - 2q]Z^2 - [4-2\delta+2\omega\varepsilon_s' - (1-\delta+\omega)q]Z \\ &+[1-\delta+\omega\varepsilon_s'].\end{aligned}$$

The proofs are summed up in Table 4 for the an-harmonic and the harmonic case.

q	ε_s	argument	result
an-harmonic: $\nu > 0$			
$]0,2[$	$> \varepsilon_\infty$	Theorem 1	stable
$]0,2]$	$= \varepsilon_\infty$	Theorem 2	stable
0	$\geq \varepsilon_\infty$	G form	stable
2	$\geq \varepsilon_\infty$	sub-polynomial	stable
harmonic: $\nu = 0$			
$]0,2[$	$> \varepsilon_\infty$	Theorem 2	stable
$]0,2]$	$= \varepsilon_\infty$	sub-polynomial	unstable
0	$\geq \varepsilon_\infty$	G form	stable
2	$\geq \varepsilon_\infty$	sub-polynomial	stable

Table 4: Proof arguments and results for the Lorentz–Joseph et al. model.

In the an-harmonic case the stability condition is $q \leq 2$ whatever $\varepsilon_s \geq \varepsilon_\infty$ is. The $\varepsilon_s = \varepsilon_\infty$ harmonic case, needs some explanation. For $q \in]0,2]$, ϕ_0 may be cast as the product of two second order polynomials. The roots are two couples of conjugate complex roots of modulus 1. For the specific value $q = 2\omega/(1+\omega)$, which always lies in the interval $]0,2]$, the two couples degenerate in one double couple, and the associated minimal stable sub-spaces are two-dimensional. To avoid this instability one may think to bound q and say that the scheme is stable provided $q \in [0, 2\omega/(1+\omega)[$. But if we come back to the original variables, we see that this is not an upper bound on k but rather a lower bound on h, which we surely do not want. It is therefore better to avoid using Joseph et al. scheme in this very specific case, $\varepsilon_s = \varepsilon_\infty$ and $\nu = 0$, and we hope to find a better scheme for this case in the following examples.

4.2 Lorentz–Kashiwa et al. model

In [7], Kashiwa et al. close a modified version of System (9), which consists of the three first equations in System (14), by a discretization for Eq. (6), namely

$$\begin{array}{rcl}
\frac{1}{k}(B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n-\frac{1}{2}}_{j+\frac{1}{2}}) & = & -\frac{1}{h}(E^n_{j+1} - E^n_j), \\
\frac{\varepsilon_0\varepsilon_\infty}{k}(E^{n+1}_j - E^n_j) & = & -\frac{1}{\mu_0 h}(B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n+\frac{1}{2}}_{j-\frac{1}{2}}) - \frac{1}{k}(P^{n+1}_j - P^n_j), \\
\frac{1}{k}(P^{n+1}_j - P^n_j) & = & \frac{1}{2}(J^{n+1}_j + J^n_j), \\
\frac{1}{k}(J^{n+1}_j - J^n_j) & = & -\frac{\nu}{2}(J^{n+1}_j + J^n_j) + \frac{\omega_1^2(\varepsilon_{\rm s} - \varepsilon_\infty)\varepsilon_0}{2}(E^{n+1}_j + E^n_j) \\
 & & -\frac{\omega_1^2}{2}(P^{n+1}_j + P^n_j).
\end{array} \qquad (14)$$

The explicit version of system (14) handles the variable

$$U^n_j = {}^t(c_\infty B^{n-\frac{1}{2}}_{j+\frac{1}{2}}, E^n_j, P^n_j/\varepsilon_0\varepsilon_\infty, kJ^n_j/\varepsilon_0\varepsilon_\infty)$$

and the amplification matrix G reads

$$\begin{pmatrix}
1 & -\lambda(e^{i\xi} - 1) & 0 & 0 \\
\frac{-\lambda(1-e^{-i\xi})(\Delta - \frac{1}{2}\omega\alpha)}{\Delta} & \frac{\Delta - q\Delta - (2-q)\frac{1}{2}\omega\alpha}{\Delta} & \frac{\omega}{\Delta} & \frac{-1}{\Delta} \\
\frac{-\lambda(1-e^{-i\xi})\frac{1}{2}\omega\alpha}{\Delta} & \frac{(2-q)\frac{1}{2}\omega\alpha}{\Delta} & \frac{\Delta-\omega}{\Delta} & \frac{1}{\Delta} \\
\frac{-\lambda(1-e^{-i\xi})\omega\alpha}{\Delta} & \frac{(2-q)\omega\alpha}{\Delta} & \frac{-2\omega}{\Delta} & \frac{2-\Delta}{\Delta}
\end{pmatrix}$$

where together with the previously defined notations, $\Delta = 1 + \delta + \omega\varepsilon'_{\rm s}/2$.

The characteristic polynomial is proportional to

$$\begin{array}{rcl}
\phi_0(Z) & = & [1 + \delta + \frac{1}{2}\omega\varepsilon'_{\rm s}]Z^4 - [4 + 2\delta - (1 + \delta + \frac{1}{2}\omega)q]Z^3 \\
 & & +[6 - \omega\varepsilon'_{\rm s} + (\omega - 2)q]Z^2 - [4 - 2\delta - (1 - \delta + \frac{1}{2}\omega)q]Z \\
 & & +[1 - \delta + \frac{1}{2}\omega\varepsilon'_{\rm s}].
\end{array}$$

The proofs are summed up in Table 5. Both in the an-harmonic and harmonic cases, the stability condition is $q < 4$ which is much better than the previous scheme since we gain a factor 2 on k and we have no problem when $\varepsilon_{\rm s} = \varepsilon_\infty$ and $\nu = 0$ as for the previous model.

q	ε_s	argument	result
an-harmonic: $\nu > 0$			
$]0,4[$	$> \varepsilon_\infty$	Theorem 1	stable
$]0,4[$	$= \varepsilon_\infty$	Theorem 2	stable
0	$\geq \varepsilon_\infty$	G form	stable
4	$\geq \varepsilon_\infty$	eigenvectors	unstable
harmonic: $\nu = 0$			
$]0,4[$	$\geq \varepsilon_\infty$	Theorem 2	stable
0	$\geq \varepsilon_\infty$	G form	stable
4	$\geq \varepsilon_\infty$	eigenvectors	unstable

Table 5: Proof arguments and results for the Lorentz–Kashiwa et al. model.

4.3 Lorentz–Young model

In [9], System (9) is closed by a discretization for Eq. (6), namely

$$\begin{aligned} &\frac{1}{k}(P_j^{n+1} - P_j^n) = J^{n+\frac{1}{2}}, \\ &\frac{1}{k}(J_j^{n+\frac{1}{2}} - J_j^{n-\frac{1}{2}}) = -\frac{\nu}{2}(J_j^{n+\frac{1}{2}} + J_j^{n-\frac{1}{2}}) \\ &\qquad\qquad +\omega_1^2(\varepsilon_\mathrm{s} - \varepsilon_\infty)\varepsilon_0 E_j^n - \omega_1^2 P_j^n. \end{aligned} \tag{15}$$

The explicit version of System (9)–(15) handles once more the variable

$$U_j^n = {}^t(c_\infty B_{j+\frac{1}{2}}^{n-\frac{1}{2}}, E_j^n, P_j^n/\varepsilon_0\varepsilon_\infty, kJ_j^n/\varepsilon_0\varepsilon_\infty)$$

and the amplification matrix G reads

$$\begin{pmatrix} 1 & -\lambda(e^{i\xi}-1) & 0 & 0 \\ -\lambda(1-e^{-i\xi}) & \frac{(1-q)(1+\delta)-2\omega\alpha}{1+\delta} & \frac{2\omega}{1+\delta} & -\frac{1-\delta}{1+\delta} \\ 0 & \frac{2\omega\alpha}{1+\delta} & \frac{1+\delta-2\omega}{1+\delta} & \frac{1-\delta}{1+\delta} \\ 0 & \frac{2\omega\alpha}{1+\delta} & \frac{-2\omega}{1+\delta} & \frac{1-\delta}{1+\delta} \end{pmatrix}$$

The characteristic polynomial is proportional to

$$\begin{aligned} \phi_0(Z) \;=\; & [1+\delta]Z^4 - [4+2\delta-2\omega\varepsilon_\mathrm{s}' - (1+\delta)q]Z^3 \\ & +2[3-2\omega\varepsilon_\mathrm{s}' + (\omega-1)q]Z^2 \\ & -[4-2\delta-2\omega\varepsilon_\mathrm{s}' - (1-\delta)q]Z + [1-\delta]. \end{aligned}$$

The proofs are summed up in Table 6. This scheme combines three drawbacks we have already encountered. First as for the Debye model, there is an extra condition on the time step: $\omega < 2/(2\varepsilon'_s - 1)$. This will have to be compared to the condition on q for physical examples. Second, as for the Lorentz–Joseph et al. scheme we need a twice smaller k than for raw Maxwell equations: $q \leq 2$ instead of $q \leq 4$. Last, and also as for the Lorentz-Joseph et al. model, the $\varepsilon_s = \varepsilon_\infty$ and $\nu = 0$ leads to an instability. This is exactly the same story. This time $q = 2\omega$ leads to double couples of conjugate complex roots of modulus 1, with two-dimensional minimal stable sub-spaces. If $\omega < 1$ this value of q is however never reached, but $\omega < 1$ is a stronger assumption than $\omega < 2/(2\varepsilon'_s - 1)$. We will see what this amounts to in numerical applications.

q	ε_s	ω	argument	result
an-harmonic: $\nu > 0$				
$]0, 2[$	$> \varepsilon_\infty$	$\leq \frac{2}{2\varepsilon'_s-1}$	Theorem 1	stable
2	$> \varepsilon_\infty$	$< \frac{2}{2\varepsilon'_s-1}$		
$]0, 2]$	$= \varepsilon_\infty$	< 2	Theorem 2	stable
$]0, 2]$	$= \varepsilon_\infty$	$= 2$	sub-polynomial	stable
2	$> \varepsilon_\infty$	$= \frac{2}{2\varepsilon'_s-1}$	Theorem 2	stable
0	$\geq \varepsilon_\infty$	$\leq \frac{2}{2\varepsilon'_s-1}$	G form	stable
harmonic: $\nu = 0$				
$]0, 2[$	$> \varepsilon_\infty$	$\leq \frac{2}{2\varepsilon'_s-1}$	Theorem 2	stable
2	$> \varepsilon_\infty$	$< \frac{2}{2\varepsilon'_s-1}$		
$]0, 2]$	$= \varepsilon_\infty$	< 2	eigenvectors	unstable
$]0, 2]$	$= \varepsilon_\infty$	$= 2$	Theorem 2	stable
2	$> \varepsilon_\infty$	$= \frac{2}{2\varepsilon'_s-1}$	eigenvectors	unstable
0	$> \varepsilon_\infty$	$\leq \frac{2}{2\varepsilon'_s-1}$	G form	stable
0	$= \varepsilon_\infty$	$< \frac{2}{2\varepsilon'_s-1}$		
0	$= \varepsilon_\infty$	$= \frac{2}{2\varepsilon'_s-1}$	eigenvectors	unstable

Table 6: Proof arguments and results for the Lorentz–Young model.

4.4 Conclusion for one-dimensional Lorentz schemes

We can summarize all our results for Lorentz schemes in Table 7. We chose not to translate the result for the Young scheme for $\varepsilon_s = \varepsilon_\infty$ as a condition on h ($q < 2\omega$) but as a condition on k ($\omega < 1$, and therefore $q = 2\omega$ is not reached).

For the harmonic Young scheme if $\varepsilon_{\mathrm{s}} > \varepsilon_\infty$ the condition is slightly better since $q = 2$ and $\omega < 2/(2\varepsilon'_{\mathrm{s}} - 1)$, or $q < 2$ and $\omega = 2/(2\varepsilon'_{\mathrm{s}} - 1)$ also yield stable schemes.

Contrarily to Debye materials, for which Joseph et al. model and Young model compete, the Kashiwa et al. model seems to overcome others for Lorentz material. First, there is a gain in CFL condition $q < 4$ is twice better as $q \leq 2$, second, there are no instabilities for limiting values of the physical coefficients and last there are no extra condition on the time step. In practice, an extra condition is however needed to account for the dynamics of the Lorentz equation, but not for stability reasons.

However we can compare the relative strength of the different conditions on k for Joseph et al. and Young models. The values used in [1] are $\varepsilon_\infty = 1$, $\varepsilon_{\mathrm{s}} = 2.25$, $\omega_1 = 4\,10^{16}\,\mathrm{rad\,s^{-1}}$ and $\nu = 0.56\,10^{16}\,\mathrm{rad\,s^{-1}}$. Condition $\omega \leq 2/\sqrt{2\varepsilon'_{\mathrm{s}} - 1}$ comes to $k \leq 2.7\,10^{-17}\,\mathrm{s}$ which is very small and corresponds to $h = 1.13\,1^{-8}\,\mathrm{m}$ in the $q < 2$ condition. This space step is more than sufficient to discretize optical waves. For such a material the extra condition imposed by the Joseph et al. scheme is stronger than the basic CFL condition. The Kashiwa et al. model is then more advisable.

In [9] there is a totally different material for which $\varepsilon_\infty = 1.5$, $\varepsilon_{\mathrm{s}} = 3$, $\omega_1 = 2\pi\,5\,10^{10}\,\mathrm{rad\,s^{-1}}$ and $\nu = 10^{10}\,\mathrm{rad\,s^{-1}}$ (these round values certainly refer to a model material). In this case $\omega \leq 2/\sqrt{2\varepsilon'_{\mathrm{s}} - 1}$ comes to $k \leq 3.6\,10^{-12}\,\mathrm{s}$ which corresponds to $h = 1.9\,1^{-3}\,\mathrm{m}$ in the $q < 2$ condition. For this material condition $q < 2$ is the strongest for optical waves. The Kashiwa et al. model is however more advisable, since it allows $q < 4$ instead of $q \leq 2$.

The results obtained in [1] where obtained for our first cited material and for Joseph et al. and Kashiwa et al. models. He observed instabilities for $\xi > \frac{\pi}{2}$. We note that if $\xi \leq \frac{\pi}{2}$ then $\sin(\xi/2) \leq 1/\sqrt{2}$ and $q \leq 2$ instead of $q \leq 4$. This is exactly our result. He found also the Kashiwa et al. scheme to stable for $q \leq 4$.

5 Two-dimensional results

In a two-dimensional context where unknowns depend only on space variables x and y, Maxwell system may be split in two decoupled systems corresponding to the transverse electric (TE) (B_x, B_y, E_z) and the transverse magnetic (TM) (B_z, E_x, E_y) polarizations. In the one-dimensional case, Maxwell–Debye equations were represented by three equations and Maxwell–Lorentz by four equations. In the TE polarization, one more Faraday equa-

Scheme		dimension 1
an-harmonic: $\nu > 0$, and $\varepsilon_s \geq \varepsilon_\infty$		
Joseph	$q \leq 2$	$k \leq \frac{h}{\sqrt{2}c_\infty}$
Kashiwa	$q < 4$	$k < \frac{h}{c_\infty}$
Young	$q \leq 2$, $\omega \leq \frac{2}{2\varepsilon'_s - 1}$	$k \leq \min(\frac{h}{\sqrt{2}c_\infty}, \frac{2}{\omega_1\sqrt{2\varepsilon'_s - 1}})$
harmonic: $\nu = 0$, and $\varepsilon_s > \varepsilon_\infty$		
Joseph	$q \leq 2$	$k \leq \frac{h}{\sqrt{2}c_\infty}$
Kashiwa	$q < 4$	$k < \frac{h}{c_\infty}$
Young	$q < 2$, $\omega < \frac{2}{2\varepsilon'_s - 1}$	$k < \min(\frac{h}{\sqrt{2}c_\infty}, \frac{2}{\omega_1\sqrt{2\varepsilon'_s - 1}})$
harmonic: $\nu = 0$, and $\varepsilon_s = \varepsilon_\infty$		
Joseph	$q < \frac{2\omega}{1+\omega}$	condition on h
Kashiwa	$q < 4$	$k < \frac{h}{c_\infty}$
Young	$q < 2$, $\omega < 1$	$k < \min(\frac{h}{\sqrt{2}c_\infty}, \frac{\sqrt{2}}{\omega_1})$

Table 7: Stability of an-harmonic and harmonic Lorentz models for $\varepsilon_s > \varepsilon_\infty$ and $\varepsilon_s > \varepsilon_\infty$.

tion is added and we have four equations for Maxwell–Debye and five equations for Maxwell–Lorentz. In the TM polarization for the Maxwell–Debye model, one Ampère equation and one Debye equation have to be added, leading to five equations systems. For the Maxwell–Lorentz model, there are one Ampère equation and two Lorentz equations more, and the system consists of seven equations.

The principle of the stability analysis is exactly the same, but we now have larger polynomials to study. A small miracle however happens: one-dimensional polynomials are a factor in two-dimensional polynomials. More precisely we now denote by h_x and h_y the space steps in the x- and y-directions respectively and by q the quantity

$$q = q_x + q_y = 4c_\infty^2 \left(\frac{k^2}{h_x^2} \sin^2(\xi_x/2) + \frac{k^2}{h_y^2} \sin^2(\xi_y/2) \right)$$

(recall $q = 4c_\infty^2 \frac{k^2}{h_x^2} \sin^2(\xi_x/2)$ in 1D). Then in the two-dimensional TE polarization

$$\phi_0^{2D,TE}(Z) = [Z - 1]\phi_0^{1D}(Z),$$

for all the Maxwell–Debye and Maxwell-Lorentz schemes we study here. This could be a problem, if 1 is already a root of $\phi_0^{1D}(Z)$, i.e. when $q = 0$, but it happens that it is never a problem: minimal stable sub-spaces are always one-dimensional. In the TM polarization, the same factorization occurs but the remaining polynomial is slightly more complicated, namely

$$\phi_0^{2D,TM}(Z) = [Z-1]\psi_0(Z)\phi_0^{1D}(Z),$$

where $\psi_0(Z)$ is equal to:
– Debye–Joseph et al. model

$$[(1+\delta\varepsilon_{\rm s}')Z - (1-\delta\varepsilon_{\rm s}')].$$

– Debye–Young model

$$[(1+\alpha)(1+\delta\alpha)Z - (1-\alpha)(1-\delta\alpha)].$$

– Lorentz–Joseph et al. model

$$[(1+\delta+\omega\varepsilon_{\rm s}')Z^2 - 2Z + (1-\delta+\omega\varepsilon_{\rm s}')].$$

- Lorentz–Kashiwa et al. model

$$[(1+\delta+\frac{1}{2}\omega\varepsilon_{\rm s}')Z^2 - (2-\omega\varepsilon_{\rm s}')Z + (1-\delta+\frac{1}{2}\omega\varepsilon_{\rm s}')].$$

– Lorentz–Young model

$$[(1+\delta)Z^2 - 2(1-\omega\varepsilon_{\rm s}')Z + (1-\delta)].$$

As for the TE polarization the extra eigenvalue 1 is never a source of instability. The other extra eigenvalues always lie inside or on the unit circle (conjugate complex roots). The only problem is when modulus 1 eigenvalues are also eigenvalues of the one-dimensional polynomial. This only occurs for the Lorentz-Joseph et al. scheme is $\varepsilon_{\rm s} = \varepsilon_\infty$, and $q = 2\omega/(1+\omega)$, which is a resonant value we have already pointed out in the harmonic case for this scheme.

We shall not duplicate Tables 3 and 7 for two-dimensional models. If $h_x = h_y \equiv h$, condition $q \le 4$ becomes $k \le h/(\sqrt{2}c_\infty)$ and condition $q \le 2$ becomes $k \le h/(2c_\infty)$ in the physical variables. Besides, Lorentz–Joseph et al. model which was leading to a lower bound on h in the harmonic case, leads also to such a bound in the an-harmonic case. These are the only differences with Tables 3 and 7.

6 Conclusion

We have studied a class of FD–TD schemes for dispersive materials based on the Yee scheme for Maxwell equations and compared them from the stability point of view. This study was inspired by Petropoulos [1] who performs the same analysis but using specific values for the physical and numerical constants and using numeric routines to locate eigenvalues of the amplification matrix. Here we have general results which gives you the constraint on numerical constants (k and h) for any Debye or Lorentz material. Our results confirm those of Petropoulos.

For usual Debye media, both studied schemes are stable under the same conditions as the Yee scheme, ensuring also, if applied to optical waves, a fine discretization of the Debye equation. Among the studied schemes for Lorentz media, Kashiwa et al. model clearly ranks first as far as stability is concerned., Its stability condition is also that of the Yee scheme. However to take properly into account the Lorentz model, a smaller time step may have to be chosen, independently of stability issues. Such results have been proved for 1D and 2D models. The 3D case, which is much more tedious, is being studied and analogous results are expected.

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