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# 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 has been analyzed in [P. Petropoulos, *Stability and phase error analysis of FD–TD in dispersive dielectrics*, IEEE Trans. Antennas Propag., 42 (1994), pp. 62–69], 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 [P. Petropoulos, *Stability and phase error analysis of FD–TD in dispersive dielectrics*, IEEE Trans. Antennas Propag., 42 (1994), pp. 62–69]. To make this approach tractable for two-dimensional and three-dimensional models, we have developed a computer algebra environment which has a wider range of applicability.

**Key words.** stability analysis, Maxwell–Debye, Maxwell–Lorentz

**AMS subject classifications.** 65M06, 65M12, 78M20

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## 1. Introduction.

To describe the propagation of an electromagnetic wave through a dispersive medium, some extensions of Maxwell equations are used. They involve time differential equations which account 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 (the Debye and Lorentz models) which are addressed in [10] in view of specific applications to the interaction of an electromagnetic wave with a human body. In [10], specific values for the physical and numerical constants are chosen and numeric calculations are performed to conclude stability or not. A survey of numerical couplings between Maxwell equations and various matter models may be found in [16], where stability conditions are given for Maxwell–Debye models, but there is no proof for some of them, and Maxwell–Lorentz formulae are considered too complex to be studied. In contrast with these two references, we are able to treat any medium which is described by these models. To this end we use von Neumann analysis.

### 1.1. Maxwell–Debye and Maxwell–Lorentz models.

In our context (no magnetization) we use different formulations of Maxwell equations where Faraday equations always read

$$\partial_t \mathbf{B}(t,\mathbf{x}) = -\operatorname{curl} \mathbf{E}(t,\mathbf{x}), \tag{1.1}$$

where $\mathbf{x} \in \mathbb{R}^N$. On the contrary, the Ampère equation may be cast using variables $\mathbf{B}$ and $\mathbf{D}$:

$$\partial_t \mathbf{D}(t,\mathbf{x}) = \frac{1}{\mu_0} \operatorname{curl} \mathbf{B}(t,\mathbf{x}); \tag{1.2a}$$

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or the polarization $\mathbf{P}$:

$$\varepsilon_0\varepsilon_\infty\partial_t\mathbf{E}(t,\mathbf{x}) = \frac{1}{\mu_0}\operatorname{curl}\mathbf{B}(t,\mathbf{x}) - \partial_t\mathbf{P}(t,\mathbf{x}), \tag{1.2b}$$

where $\mathbf{P}(t,\mathbf{x}) = \mathbf{D}(t,\mathbf{x}) - \varepsilon_0\varepsilon_\infty\mathbf{E}(t,\mathbf{x})$ and $\varepsilon_\infty$ is the relative infinite frequency permittivity. Denoting by $\mathbf{J}$ the time derivative of $\mathbf{P}$, we also have

$$\varepsilon_0\varepsilon_\infty\partial_t\mathbf{E}(t,\mathbf{x}) = \frac{1}{\mu_0}\operatorname{curl}\mathbf{B}(t,\mathbf{x}) - \mathbf{J}(t,\mathbf{x}). \tag{1.2c}$$

The system of Faraday and Ampère equations is closed by a linear constitutive law,

$$\mathbf{D}(t,\mathbf{x}) = \varepsilon_0\varepsilon_\infty\mathbf{E}(t,\mathbf{x}) + \varepsilon_0\int_{-\infty}^{t}\mathbf{E}(t-\tau,\mathbf{x})\chi(\tau)d\tau, \tag{1.3}$$

where $\chi$ is the linear susceptibility. The discretization of the integral expression (1.3) leads to recursive schemes (see, e.g., [7], [17]). However, differentiating (1.3) leads to a time differential equation for $\mathbf{D}$ which depends on the specific form of $\chi$. For a Debye medium,

$$t_{\mathrm{r}}\partial_t\mathbf{D} + \mathbf{D} = t_{\mathrm{r}}\varepsilon_0\varepsilon_\infty\partial_t\mathbf{E} + \varepsilon_0\varepsilon_{\mathrm{s}}\mathbf{E}, \tag{1.4a}$$

where $t_{\mathrm{r}} > 0$ is the relaxation time and $\varepsilon_{\mathrm{s}} \geq \varepsilon_\infty$ is the relative static permittivity. An equivalent form of (1.4a) using variable $\mathbf{P}$ is

$$t_{\mathrm{r}}\partial_t\mathbf{P} + \mathbf{P} = \varepsilon_0(\varepsilon_{\mathrm{s}} - \varepsilon_\infty)\mathbf{E}, \tag{1.4b}$$

which can be coupled with the Ampère equation cast as (1.2b). For a Lorentz medium with one resonant frequency $\omega_1$, we likewise have

$$\partial_t^2\mathbf{D} + \nu\partial_t\mathbf{D} + \omega_1^2\mathbf{D} = \varepsilon_0\varepsilon_\infty\partial_t^2\mathbf{E} + \varepsilon_0\varepsilon_\infty\nu\partial_t\mathbf{E} + \varepsilon_0\varepsilon_{\mathrm{s}}\omega_1^2\mathbf{E}, \tag{1.5a}$$

where $\nu \geq 0$ is a damping coefficient, or, equivalently,

$$\partial_t^2\mathbf{P} + \nu\partial_t\mathbf{P} + \omega_1^2\mathbf{P} = \varepsilon_0(\varepsilon_{\mathrm{s}} - \varepsilon_\infty)\omega_1^2\mathbf{E}. \tag{1.5b}$$

**1.2. Yee-based numerical schemes.** A classical and very efficient way to compute the Maxwell equations is the Yee scheme [14]. We restrict our study to existing Yee-based schemes. 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 (1.4a) to (1.5b) (see [5], [4], [15]). Other space discretizations may be found in the literature in the context of Maxwell–Debye and Maxwell–Lorentz equations; see, e.g., [3] for pseudo-spectral schemes or [12] for finite element–time domain (FE–TD) schemes.

The Yee scheme consists of discretizing $\mathbf{E}$ and $\mathbf{B}$ on staggered grids in space and time. This allows one 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 consider only the dependence in the space variable $z$; classically, two polarizations for the field may be decoupled. For example, the transverse electric polarization involves only $E \equiv E_x$ and $B \equiv B_y$. The discretized variables are $E_j^n \simeq E(nk, jh)$ (and similar

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notations for $D \equiv D_x$) and $B^{n+\frac{1}{2}}_{j+\frac{1}{2}} \simeq B((n+\frac{1}{2})k, (j+\frac{1}{2})h)$, and the Yee scheme for the Maxwell equation reads

$$\frac{B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n-\frac{1}{2}}_{j+\frac{1}{2}}}{k} = -\frac{E^n_{j+1} - E^n_j}{h}, \tag{1.6}$$

coupled with one of the following:

$$\frac{D^{n+1}_j - D^n_j}{k} = -\mu_0 \frac{B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{h}, \tag{1.7a}$$

$$\varepsilon_0\varepsilon_\infty \frac{E^{n+1}_j - E^n_j}{k} = -\mu_0 \frac{B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{h} - \frac{P^{n+1}_j - P^n_j}{k}, \tag{1.7b}$$

$$\varepsilon_0\varepsilon_\infty \frac{E^{n+1}_j - E^n_j}{k} = -\mu_0 \frac{B^{n+\frac{1}{2}}_{j+\frac{1}{2}} - B^{n+\frac{1}{2}}_{j-\frac{1}{2}}}{h} - J^{n+\frac{1}{2}}_j. \tag{1.7c}$$

Usual Maxwell equations consist of taking $J^{n+\frac{1}{2}}_j \equiv 0$ in (1.7c) or, equivalently, $D^n_j = \varepsilon_0\varepsilon_\infty E^n_j$ in (1.7a) and lead 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, then the CFL condition reads $c_\infty k \le h/\sqrt{N}$.

**1.3. Scheme naming.** Since we deal with many schemes, we have to distinguish between them and name them. Numbers or names of first contributor(s) are not very meaningful, and we prefer here to have a descriptive name. Our description gives both the variables used (e.g., coupling (1.2a) and (1.4a) uses variables **B**, **E**, and **D**) and the location of discretized variables. Space occurs only as a parameter in Debye or Lorentz equations. To avoid interpolation, the reasonable choice is to always locate variables **D**, **P**, and **J** on the same space grid as **E**. The different schemes therefore differ only in the time location of variables: in (1.7a) and (1.7b) integer times are chosen; in (1.7c) half-integer times are chosen.

Our naming convention is the following: we separate variables at half-integer times from variables at integer times by an underscore sign, e.g., "B_ED" when coupling (1.6) and (1.7a). In Table 1.1 we give the correspondence between the article where the schemes have been derived first, the terminology of the survey [16] and our description.

Table 1.1
*Correspondence between different namings.*

| Contributor(s) | Name in [16] | Description | Name in [16] | Description |
|---|---|---|---|---|
| | Debye | | Lorentz | |
| Joseph et al. [4] | D-DIM 3 | B_ED | L-DIM 3 | B_ED |
| Kashiwa et al. [5] | D-DIM 2 | B_EP | L-DIM 2 | B_EPJ |
| Young [15] | D-DIM 1 | BP_E | L-DIM 1 | BJ_EP |

**1.4. Outline.** The von Neumann stability analysis is recalled in section 2. We also describe the sketch of our proofs which is common for all of the schemes. In section 3, three one-dimensional direct integration schemes for Debye media are presented and analyzed, carefully pointing out the physical properties needed to ensure stability and the specific cases which have to be handled separately. Numerical applications to

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physical media are also given. The same point of view is carried out for Lorentz media in section 4. To address two- and three-dimensional schemes which have too many variables to compute by hand, we have developed a computer algebra environment based on MAPLE, which is described in section 5. Two- and three dimensional results are given in section 6.

## 2. Principles of the von Neumann analysis.

The von Neumann analysis allows one 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 [13].

### 2.1. Schur and simple von Neumann polynomials.

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

DEFINITION 2.1. *A polynomial is a Schur polynomial if all its roots, $r$, satisfy $|r| < 1$.*

DEFINITION 2.2. *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 has a high degree or 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, we construct a sequence of polynomials of decreasing degree. Let $\phi$ be written as

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

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

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

Given a polynomial $\phi_0$, 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 $\phi_m \not\equiv 0$.

THEOREM 2.3. *A polynomial $\phi_m$ is a Schur polynomial of exact degree $d$ if and only if $\phi_{m+1}$ is a Schur polynomial of exact degree $d-1$ and $|\phi_m(0)| \leq |\phi_m^*(0)|$.*

THEOREM 2.4. *A polynomial $\phi_m$ is a simple von Neumann polynomial if and only if*

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

*or*

- *$\phi_{m+1}$ is identically zero and $\phi_m'$ is a Schur polynomial.*

The main ingredient in the proof of both theorems is the Rouché theorem (see [9], [13]). To analyze $\phi_0$, at each step $m$, conditions should be checked (leading coefficient is nonzero, $|\phi_m(0)| \leq |\phi_m^*(0)|, \ldots$) 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. We can thus assume that the scheme handles a single vector-valued 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

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but only on the ratio $h/k$. Let $\phi_0$ be the characteristic polynomial of $G$; then we have a sufficient stability condition.

THEOREM 2.5. *A sufficient stability condition is that $\phi_0$ 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, then $U^n = G^n U^0$ and stability is also the boundedness of $(G^n)_{n\in\mathbb{N}}$. If the eigenvalues of $G$, i.e., the roots $r$ of $\phi_0$, 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. Consider, for example, the case 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 $(G^n)_{n\in\mathbb{N}}$. It is clearly a property of the amplification matrix and not of its characteristic polynomial. If the dimension of eigensubspace associated with a root is equal to its multiplicity, then $G^n$ is bounded (an example for this is the identity: $\mathrm{Id}^n = \mathrm{Id}$ remains bounded). In the opposite case $G^n$ grows linearly. A paradigm for this is

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}^n = \begin{pmatrix} 1 & n \\ 0 & 1 \end{pmatrix},$$

which grows linearly with iterations, and only one eigenvector can be found. Such cases (which occur for our schemes) should therefore be handled specifically.

We will stick here to locating roots in the unit circle. Another way has already been developed in, e.g., [6], [11]. It consists of using a conformal map to locate roots in the left half-plane. This changes the problem in a Routh–Hurwitz problem, which reads as a list of sufficient conditions for the characteristic polynomial to be von Neumann ($|r| \le 1$). This has been implemented in the FIDE REDUCE package.

**2.3. Sketch of proofs.** In the next sections, we will not give the proofs, but only list in tables 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 [1] for space dimensions 1 and 2. The three-dimensional case has been performed *via* computer algebra simulations [2].

Usually the coupled system is given in an implicit form. The first step consists of writing it in an explicit form. This yields the amplification matrix $G$. Then we compute its characteristic polynomial $\phi_0$. In order to perform a von Neumann analysis, we compute the series $(\phi_m)$. In the general case, under the assumption that the stability condition cannot be better than Yee's, we can apply either Theorem 2.3 (*Theorem* 2.3 argument) or Theorem 2.4 (*Theorem* 2.4 argument), checking estimates at each level until $\phi_m$ is a one degree polynomial. Special cases arise when $\varepsilon_{\mathrm{s}} = \varepsilon_\infty$, $\sin(\xi/2) = 0$ or $\pm 1$, and sometimes for limit values of physical coefficients. In these cases, different points of view have to be considered:

- Theorem 2.4 has to be used instead of Theorem 2.3.
- Some eigenvalues lie on the unit circle (mostly $\pm 1$ or $\pm i$). Polynomial $\phi_0$ is at best a simple von Neumann polynomial and we have to study the other eigenvalues which are roots of a lower degree polynomial (*subpolynomial* argument).
- Some eigenvalues lie on the unit circle and are not simple. Besides the study of the other eigenvalues (*subpolynomial* argument), we have to compare the

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multiplicity of the root to the number of eigenvectors found. If they are equal (stable case), then this is usually checked directly on the form of matrix $G$ ($G$ *form* argument). The unstable case necessitates the computation of eigenvectors (*eigenvectors* argument).

If $\varepsilon_s = \varepsilon_\infty$, then Maxwell equations decouple from the other equations. We study this limit as a hint of how the numerical scheme may behave when $\varepsilon_s$ is very close to $\varepsilon_\infty$. For the same reason, we will study the undamped oscillator ($\nu = 0$) for Lorentz media.

**3. Debye media.** We address successively the three discretizations of Maxwell–Debye equations mentioned in Table 1.1.

**3.1. Debye B_ED scheme.** In [4], Joseph, Hagness, and Taflove close system (1.6)–(1.7a) by a discretization for (1.4a), namely

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

The resulting system may be cast in an explicit form which handles the variable ($^t$ denotes transposition)

$$U_j^n=\left(c_\infty B_{j+\frac12}^{n-\frac12},E_j^n,D_j^n/\varepsilon_0\varepsilon_\infty\right)^t,$$

and the amplification matrix $G$ reads

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

where $\lambda = c_\infty k/h$ is the CFL constant, $\delta = k/2t_\mathrm{r} > 0$ is the normalized time step, and $\eta_\mathrm{s} = \varepsilon_\mathrm{s}/\varepsilon_\infty \geq 1$ 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

$$\phi_0(Z)=[1+\delta\eta_\mathrm{s}]Z^3-[3+\delta\eta_\mathrm{s}-(1+\delta)q]Z^2+[3-\delta\eta_\mathrm{s}-(1-\delta)q]Z-[1-\delta\eta_\mathrm{s}].$$

The proof arguments are summed up in Table 3.1, and we deduce that the stability condition is $q \leq 4$ if $\varepsilon_\mathrm{s} > \varepsilon_\infty$ and $q < 4$ if $\varepsilon_\mathrm{s} = \varepsilon_\infty$.

Table 3.1
*Proof arguments and results for the Debye B_ED and B_EP schemes.*

| $q$ | $\varepsilon_\mathrm{s}$ | Argument | Result |
|---|---|---|---|
| $]0,4[$ | $>\varepsilon_\infty$ | Theorem 2.3 | stable |
| $]0,4[$ | $=\varepsilon_\infty$ | Theorem 2.4 | stable |
| 0 | $\geq\varepsilon_\infty$ | $G$ form | stable |
| 4 | $>\varepsilon_\infty$ | Theorem 2.4 | stable |
| 4 | $=\varepsilon_\infty$ | eigenvectors | unstable |

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**3.2. Debye B_EP scheme.** In [5], Kashiwa, Yoshida, and Fukai close system (1.6)–(1.7b) by a discretization for (1.4b):

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

The system now handles the variable

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

the amplification matrix $G$ reads

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

and the characteristic polynomial is proportional to the same polynomial as for the B_ED scheme. All proofs are the same except those on matrix $G$ directly, but even in these cases the conclusions are the same. Table 3.1 is also valid for the B_EP scheme.

**3.3. Debye BP_E scheme.** In [15], Young chooses to close system (1.6)–(1.7c) by two discretizations for (1.4b), namely

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

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

Although $J_j^{n+\frac{1}{2}}$ is used for the computations, this not a genuine variable for the full system which handles the variable

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

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 notations as above and $\alpha = \eta_{\mathrm{s}} - 1 \geq 0$. The characteristic polynomial is proportional to

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

Table 3.2 gathers the different arguments used. The stability condition is $q \leq 4$ and $\delta \leq 1$ if $\varepsilon_{\mathrm{s}} > \varepsilon_\infty$ and $q < 4$ if $\varepsilon_{\mathrm{s}} = \varepsilon_\infty$.

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TABLE 3.2
*Proof arguments and results for the Debye BP_E scheme.*

| $q$ | $\varepsilon_s$ | $\delta$ | Argument | Result |
|---|---|---|---|---|
| $]0,4]$ | $> \varepsilon_\infty$ | $]0,1[$ | Theorem 2.3 | stable |
| $]0,4[$ | $= \varepsilon_\infty$ | $> 0$ | Theorem 2.4 | stable |
| 0 | $\geq \varepsilon_\infty$ | $> 0$ | $G$ form | stable |
| $]0,4]$ | $> \varepsilon_\infty$ | 1 | subpolynomial | stable |
| 4 | $= \varepsilon_\infty$ | $> 0$ | eigenvectors | unstable |

**3.4. Conclusion for one-dimensional Debye schemes.** If $\varepsilon_s > \varepsilon_\infty$, then the pure CFL condition $q \leq 4$ is the same for both models. It is exactly the condition for Maxwell equations. However, the BP_E scheme necessitates another condition, $\delta \leq 1$, which corresponds to a sufficient discretization of Debye equation (1.4b). Even if we are interested here in stability properties, such conditions are to be considered to ensure equations to be correctly taken into account. Results are given in physical variables in Table 3.3.

TABLE 3.3
*Stability of Debye models for $\varepsilon_s > \varepsilon_\infty$ and $\varepsilon_s = \varepsilon_\infty$.*

| Scheme | | Dimension 1 | | Dimension 1 |
|---|---|---|---|---|
| | $\varepsilon_s > \varepsilon_\infty$ | | $\varepsilon_s = \varepsilon_\infty$ | |
| B_ED or B_EP | $q \leq 4$ | $k \leq h/c_\infty$ | $q < 4$ | $k < h/c_\infty$ |
| BP_E | $q \leq 4$, $\delta \leq 1$ | $k \leq \min(h/c_\infty, 2t_r)$ | $q < 4$ | $k < h/c_\infty$ |

To compare conditions on $q$ and $\delta$, let us consider a simple physical case. We assume that a matter with $\varepsilon_\infty = 1$ (and thus $c_\infty \simeq 3 \times 10^8\,\mathrm{m\,s^{-1}}$) is lighted by a wave of, say, wavelength 1 cm. The space step $h$ has to be smaller than this wavelength, and therefore $q < 4$ reads at least $k < \frac{1}{3} \times 10^{-10}\,\mathrm{s}$. In a Debye medium, relaxation times $t_r$ are of the order of a picosecond (or even a nanosecond) which maybe of the same order than the previous bound. A typical example is water, for which $\varepsilon_\infty = 1.8$, $\varepsilon_s = 81.0$, and $t_r = 9.4 \times 10^{-12}\,\mathrm{s}$ [17]. Condition $k \leq 2t_r$ comes to $k \leq 1.88 \times 10^{-11}\,\mathrm{s}$. Condition $q \leq 4$ yields a similar condition if $h = 4.2 \times 10^{-3}\,\mathrm{m}$. For a very coarse space grid and with the BP_E scheme, the CFL condition comes from $k \leq 2t_r$; otherwise, for a fine grid and/or B_ED or B_EP schemes, it comes from $q \leq 4$.

A quite different material is, for example, the 0.25-dB loaded foam given in [8] for which $\varepsilon_\infty = 1.01$, $\varepsilon_s = 1.16$, and $t_r = 6.497 \times 10^{-10}\,\mathrm{s}$. Condition $k \leq 2t_r$ comes to $k \leq 1.3 \times 10^{-9}\,\mathrm{s}$ and $q \leq 4$ yields a similar condition if $h = 3.9 \times 10^{-1}\,\mathrm{m}$. In practice $h$ has to be smaller to describe a wave with 1 cm wavelength, and the stability condition for this foam is $q < 4$ for both schemes.

In conclusion, the stability condition may depend on the material in classical applications, leading us to prefer the B_ED scheme, when $t_r$ is small (picosecond). The result announced in [10] was $q \leq 4$ for the B_ED scheme and for water, which is consistent with our result.

**4. Lorentz media.** We now address the three discretizations of Maxwell–Lorentz equations mentioned in Table 1.1.

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

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**4.1. Lorentz B_ED scheme.** In [4], system (1.6)–(1.7a) is closed by a discretization for (1.5a), namely

$$\varepsilon_0\varepsilon_\infty\frac{E_j^{n+1}-2E_j^n+E_j^{n-1}}{k^2}+\nu\varepsilon_0\varepsilon_\infty\frac{E_j^{n+1}-E_j^{n-1}}{2k}+\varepsilon_0\varepsilon_s\omega_1^2\frac{E_j^{n+1}+E_j^{n-1}}{2}$$
$$=\frac{D_j^{n+1}-2D_j^n+D_j^{n-1}}{k^2}+\nu\frac{D_j^{n+1}-D_j^{n-1}}{2k}+\omega_1^2\frac{D_j^{n+1}+D_j^{n-1}}{2}.$$

The explicit version of the subsequent system does not explicitly use the value of $D_j^{n-1}$, and therefore this system handles the variable

$$U_j^n=\left(c_\infty B_{j+\frac12}^{n-\frac12},E_j^n,E_j^{n-1},D_j^n/\varepsilon_0\varepsilon_\infty\right)^t.$$

The amplification matrix $G$ reads

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

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

$$\phi_0(Z)=[1+\delta+\omega\eta_s]Z^4-[4+2\delta+2\omega\eta_s-(1+\delta+\omega)q]Z^3$$
$$+[6+2\omega\eta_s-2q]Z^2-[4-2\delta+2\omega\eta_s-(1-\delta+\omega)q]Z+[1-\delta+\omega\eta_s].$$

The proofs are summed up in Table 4.1 for the damped and the undamped case.

Table 4.1
*Proof arguments and results for the Lorentz B_ED scheme.*

| $q$ | $\varepsilon_s$ | Argument | Result | Argument | Result |
|---|---|---|---|---|---|
| | | damped: $\nu>0$ | | undamped: $\nu=0$ | |
| $]0,2[$ | $>\varepsilon_\infty$ | Theorem 2.3 | stable | Theorem 2.4 | stable |
| $]0,2]$ | $=\varepsilon_\infty$ | Theorem 2.4 | stable | subpolynomial | unstable |
| 0 | $\geq\varepsilon_\infty$ | $G$ form | stable | $G$ form | stable |
| 2 | $\geq\varepsilon_\infty$ | subpolynomial | stable | subpolynomial | stable |

In the damped case the stability condition is $q\leq 2$ for all $\varepsilon_s\geq\varepsilon_\infty$. The $\varepsilon_s=\varepsilon_\infty$ undamped case needs some explanation. For $q\in]0,2]$, $\phi_0$ 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 with only two eigendirections, which is the unstable case. 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 the B_ED scheme in this very specific case, $\varepsilon_s=\varepsilon_\infty$ and $\nu=0$. A better scheme for this case is provided next.

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**4.2. Lorentz B_EPJ scheme.** In [5], Kashiwa, Yoshida, and Fukai close system (1.6)–(1.7b) by a discretization for (1.5b), namely

$$\frac{P_j^{n+1}-P_j^n}{k}=\frac{J_j^{n+1}+J_j^n}{2},$$
$$\frac{J_j^{n+1}-J_j^n}{k}=-\nu\frac{J_j^{n+1}+J_j^n}{2}+\omega_1^2(\varepsilon_{\rm s}-\varepsilon_\infty)\varepsilon_0\frac{E_j^{n+1}+E_j^n}{2}-\omega_1^2\frac{P_j^{n+1}+P_j^n}{2}.$$

The explicit version of the system obtained handles the variable

$$U_j^n=\left(c_\infty B_{j+\frac12}^{n-\frac12},E_j^n,P_j^n/\varepsilon_0\varepsilon_\infty,kJ_j^n/\varepsilon_0\varepsilon_\infty\right)^t,$$

and the amplification matrix $G$ reads

$$\begin{pmatrix} 1 & -\lambda(e^{i\xi}-1) & 0 & 0\\ \frac{-\lambda(1-e^{-i\xi})(\Delta-\frac12\omega\alpha)}{\Delta} & \frac{\Delta-q\Delta-(2-q)\frac12\omega\alpha}{\Delta} & \frac{\omega}{\Delta} & \frac{-1}{\Delta}\\ \frac{-\lambda(1-e^{-i\xi})\frac12\omega\alpha}{\Delta} & \frac{(2-q)\frac12\omega\alpha}{\Delta} & \frac{\Delta-\omega}{\Delta} & \frac{1}{\Delta}\\ \frac{-\lambda(1-e^{-i\xi})\omega\alpha}{\Delta} & \frac{(2-q)\omega\alpha}{\Delta} & \frac{-2\omega}{\Delta} & \frac{2-\Delta}{\Delta} \end{pmatrix},$$

where together with the previously defined notations, $\Delta=1+\delta+\omega\eta_{\rm s}/2$. The characteristic polynomial is proportional to

$$\phi_0(Z)=\left[1+\delta+\frac12\omega\eta_{\rm s}\right]Z^4-\left[4+2\delta-\left(1+\delta+\frac12\omega\right)q\right]Z^3$$
$$+[6-\omega\eta_{\rm s}+(\omega-2)q]Z^2-\left[4-2\delta-\left(1-\delta+\frac12\omega\right)q\right]Z+\left[1-\delta+\frac12\omega\eta_{\rm s}\right].$$

The proofs are summed up in Table 4.2. Both in the damped and undamped 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.

Table 4.2
*Proof arguments and results for the Lorentz B_EPJ scheme.*

| $q$ | $\varepsilon_{\rm s}$ | Argument | Result | Argument | Result |
|---|---|---|---|---|---|
| | | damped: $\nu>0$ | | undamped: $\nu=0$ | |
| $]0,4[$ | $>\varepsilon_\infty$ | Theorem 2.3 | stable | Theorem 2.4 | stable |
| $]0,4[$ | $=\varepsilon_\infty$ | Theorem 2.4 | stable | Theorem 2.4 | stable |
| 0 | $\geq\varepsilon_\infty$ | $G$ form | stable | $G$ form | stable |
| 4 | $\geq\varepsilon_\infty$ | eigenvectors | unstable | eigenvectors | unstable |

**4.3. Lorentz BJ_EP scheme.** In [15], system (1.6)–(1.7c) is closed by a discretization for (1.5b), namely

$$\frac{P_j^{n+1}-P_j^n}{k}=J^{n+\frac12},$$
$$\frac{J_j^{n+\frac12}-J_j^{n-\frac12}}{k}=-\nu\frac{J_j^{n+\frac12}+J_j^{n-\frac12}}{2}+\omega_1^2(\varepsilon_{\rm s}-\varepsilon_\infty)\varepsilon_0E_j^n-\omega_1^2P_j^n.$$

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The explicit version of the system handles the variable

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

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

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

Table 4.3

*Proof arguments and results for the Lorentz BJ_EP scheme.*

| $q$ | $\varepsilon_{\mathrm{s}}$ | $\omega$ | Argument | Result |
|---|---|---|---|---|
| damped: $\nu > 0$ | | | | |
| $]0,2[$ | $> \varepsilon_\infty$ | $\leq 2/(2\eta_{\mathrm{s}}-1)$ | Theorem 2.3 | stable |
| 2 | $> \varepsilon_\infty$ | $< 2/(2\eta_{\mathrm{s}}-1)$ | | |
| $]0,2]$ | $= \varepsilon_\infty$ | $< 2$ | Theorem 2.4 | stable |
| $]0,2]$ | $= \varepsilon_\infty$ | $= 2$ | subpolynomial | stable |
| 2 | $> \varepsilon_\infty$ | $= 2/(2\eta_{\mathrm{s}}-1)$ | Theorem 2.4 | stable |
| 0 | $\geq \varepsilon_\infty$ | $\leq 2/(2\eta_{\mathrm{s}}-1)$ | G form | stable |
| $q$ | $\varepsilon_{\mathrm{s}}$ | $\omega$ | Argument | Result |
| undamped: $\nu = 0$ | | | | |
| $]0,2[$ | $> \varepsilon_\infty$ | $\leq 2/(2\eta_{\mathrm{s}}-1)$ | Theorem 2.4 | stable |
| 2 | $> \varepsilon_\infty$ | $< 2/(2\eta_{\mathrm{s}}-1)$ | | |
| $]0,2]$ | $= \varepsilon_\infty$ | $< 2$ | eigenvectors | unstable |
| $]0,2]$ | $= \varepsilon_\infty$ | $= 2$ | Theorem 2.4 | stable |
| 2 | $> \varepsilon_\infty$ | $= 2/(2\eta_{\mathrm{s}}-1)$ | eigenvectors | unstable |
| 0 | $> \varepsilon_\infty$ | $\leq 2/(2\eta_{\mathrm{s}}-1)$ | G form | stable |
| 0 | $= \varepsilon_\infty$ | $< 2/(2\eta_{\mathrm{s}}-1)$ | | |
| 0 | $= \varepsilon_\infty$ | $= 2/(2\eta_{\mathrm{s}}-1)$ | eigenvectors | unstable |

The proofs are summed up in Table 4.3. This scheme combines three drawbacks we have already encountered. First, as for the Debye model, there is an extra condition on the time step: $\omega < 2/(2\eta_{\mathrm{s}}-1)$. This will have to be compared to the condition on $q$ for physical examples. Second, as for the Lorentz B_ED 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 B_ED scheme, the $\varepsilon_{\mathrm{s}} = \varepsilon_\infty$ and $\nu = 0$ lead 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 only two eigendirections. If $\omega > 1$, then this value of $q$ is, however, never reached. Else $q = 2\omega$ is rather a condition on $h$ and therefore not a proper stability condition. As for the Lorentz B_ED, it seems better to avoid using this scheme if $\varepsilon_{\mathrm{s}} = \varepsilon_\infty$ and $\nu = 0$.

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**4.4. Conclusion for one-dimensional Lorentz schemes.** We summarize all our results for Lorentz schemes in Table 4.4. For the undamped BJ_EP scheme, if $\varepsilon_s > \varepsilon_\infty$, then the condition is slightly better since $q = 2$ and $\omega < 2/(2\eta_s - 1)$, or $q < 2$ and $\omega = 2/(2\eta_s - 1)$ also yield stable schemes.

Contrarily to Debye materials, for which all schemes compete, the B_EPJ scheme seems to overcome others for Lorentz material. First, there is a gain in CFL condition ($q < 4$ is twice better as $q \le 2$), second, there are no instabilities for limiting values of the physical coefficients, and last, there is 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 the B_ED and BJ_EP schemes, and for optical waves of, say, wavelength $1\,\mu$m. The values used in [10] are $\varepsilon_\infty = 1$, $\varepsilon_s = 2.25$, $\omega_1 = 4 \times 10^{16}\,\mathrm{rad\,s^{-1}}$, and $\nu = 0.56 \times 10^{16}\,\mathrm{rad\,s^{-1}}$. Condition $\omega \le 2/\sqrt{2\eta_s - 1}$ comes to $k \le 2.7 \times 10^{-17}\,$s, which is very small and corresponds to $h = 1.13 \times 10^{-8}\,$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 B_ED scheme is stronger than the basic CFL condition. The B_EPJ model is then more advisable.

TABLE 4.4
*Stability of damped and undamped Lorentz models for $\varepsilon_s > \varepsilon_\infty$ and $\varepsilon_s = \varepsilon_\infty$.*

| Scheme | | Dimension 1 |
|---|---|---|
| damped: $\nu > 0$, and $\varepsilon_s \ge \varepsilon_\infty$ | | |
| B_ED | $q \le 2$ | $k \le h/\sqrt{2}c_\infty$ |
| B_EPJ | $q < 4$ | $k < h/c_\infty$ |
| BJ_EP | $q \le 2$, $\omega \le 2/(2\eta_s - 1)$ | $k \le \min(h/\sqrt{2}c_\infty, 2/\omega_1\sqrt{2\eta_s - 1})$ |
| undamped: $\nu = 0$, and $\varepsilon_s > \varepsilon_\infty$ | | |
| B_ED | $q \le 2$ | $k \le h/\sqrt{2}c_\infty$ |
| B_EPJ | $q < 4$ | $k < h/c_\infty$ |
| BJ_EP | $q < 2$, $\omega < 2/(2\eta_s - 1)$ | $k < \min(h/\sqrt{2}c_\infty, 2/\omega_1\sqrt{2\eta_s - 1})$ |
| undamped: $\nu = 0$, and $\varepsilon_s = \varepsilon_\infty$ | | |
| B_ED | $q < 2\omega/(1+\omega)$ | condition on $h$ |
| B_EPJ | $q < 4$ | $k < h/c_\infty$ |
| BJ_EP | $q < 2$, $\omega < 2/(2\eta_s - 1)$ | $k < \min(h/\sqrt{2}c_\infty, 2/\omega_1\sqrt{2\eta_s - 1})$ if $\omega > 1$; condition on $h$ else |

In [15] there is a totally different material for which $\varepsilon_\infty = 1.5$, $\varepsilon_s = 3$, $\omega_1 = 2\pi \times 5 \times 10^{10}\,\mathrm{rad\,s^{-1}}$, and $\nu = 10^{10}\,\mathrm{rad\,s^{-1}}$ (these round values certainly refer to a model material). In this case $\omega \le 2/\sqrt{2\eta_s - 1}$ comes to $k \le 3.6 \times 10^{-12}\,$s, which corresponds to $h = 1.9 \times 10^{-3}\,$m in the $q < 2$ condition. For this material condition $q < 2$ is the strongest for optical waves. The B_EPJ scheme is, however, more advisable, since it allows $q < 4$ instead of $q \le 2$.

The results obtained in [10] were obtained for our first cited material and for the B_ED and BJ_EP schemes. Petropoulos observed instabilities for $\xi > \frac{\pi}{2}$. We note that if $\xi \le \frac{\pi}{2}$, then $\sin(\xi/2) \le 1/\sqrt{2}$ and $q \le 2$ instead of $q \le 4$. This is exactly our result. He found also the B_EPJ scheme to be stable for $q \le 4$.

**5. Automation *via* computer algebra.** For a three-dimensional Lorentz medium, $\phi_0$ is typically a 12th degree polynomial with polynomial coefficients of

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degree 6 in the different parameters. The previous procedure becomes awful if made by hand. A computer algebra environment based on MAPLE has been developed specifically to automate all the computational steps which may be the source of errors [2]. It is still dedicated only to electromagnetic models but could be extended in the future to other applications.

The schemes are defined by four parameters:

1. the space dimension `Dim` (1, 2 or 3),
2. the polarization `Polar` (TE or TM in dimension 2),
3. the physical model `Model` (e.g., Debye),
4. the variables used `Formula` (e.g., `B_EP`).

Maxwell equations have been written once and for all and just have to be “called”:

```
> Faraday(Eq, Dim, Polar):
> Ampere(Eq, Dim, Polar, Formula):
```

For our applications, in the other equations space is only a parameter. Such equations are written once with no spatial dependence:

```
> NewEq := tr*(P[n+1]-P[n])/dt
         + 1/2*(P[n+1]+P[n])
         - eps0*(epss-epsinfini)*(E[n+1]+E[n])/2:
> CreateEq(Eq, NewEq, Dim, Polar):
```

and propagated to all the useful coordinates with the right indexes on the staggered grid, according to the space dimension and polarization.

Then changes of variables are automatically performed to have dimensionless variables (specific to the model), no redundant variables (specific to the scheme), and an explicit scheme in the frequency domain. This yields the amplification matrix $G$. The computation of polynomial $\phi_0$ is then performed as well as the computational part of the von Neumann analysis: computation of the sequence of polynomials and factorizations. On these forms the user of the toolbox can easily see which are the specific cases to consider separately.

The comparisons $|\phi_m(0)| \leq |\phi_m^*(0)|$ are the real difficult points from the computer algebra point of view; therefore it is necessary to evaluate the sign of a polynomial in many variables (4 for a Lorentz medium) and of total degree of order say 6 for $\phi_0$, about 10 for $\phi_1, \ldots$ knowing some variables are positive (like $\eta_s - 1$ or $\delta$) and others lie within an interval (like $q$). This is also automated:

```
> SignCheck(phi, Z, [0 < delta, 1 < etas, 0 < q, q < 4]),
```

but sometimes MAPLE does not yield a totally explicit answer. This might lead us to migrate the whole toolbox in a C code to make use of some existing softwares specific for the solving of interval arithmetic problems.

Finally, tools are defined to compare the number of eigenvectors and the multiplicity of eigenvalues in the degenerate cases.

## 6. Two- and three-dimensional results.

**6.1. Equation setting.** In a two-dimensional context where unknowns depend only on space variables $x$ and $y$, the 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 equation is added; therefore, 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 equation systems. For the

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Maxwell–Lorentz model, there is one more Ampère equation and two more Lorentz equations, so the system consists of seven equations.

In the three-dimensional context, equations do not decouple any more, and systems consist of nine equations for the Maxwell–Debye schemes and twelve equations for the Maxwell–Lorentz schemes.

The principle of the stability analysis is exactly the same, but we now have larger polynomials to study. We, however, found out that the one-dimensional polynomials (which we denote by $\phi_0^{1D}(Z)$) are a factor in two- and three-dimensional polynomials, which reduces the formal calculations. More precisely we now denote by $h_x$, $h_y$, and $h_z$ the space steps in the $x$-, $y$-, and $z$-directions, respectively, and by $q$ the quantity

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

or

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

according to the space dimension (recall $q = 4c_\infty^2 \frac{k^2}{h_x^2} \sin^2(\xi_x/2)$ in one dimension).

**6.2. Results.** In the two-dimensional TE polarization, the characteristic polynomial reads

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

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., if $q = 0$, but it happens that it is never a problem: minimal stable subspaces 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 B_ED and B_EP: $[(1+\delta\eta_{\mathrm{s}})Z - (1-\delta\eta_{\mathrm{s}})]$,
- Debye BP_E: $[(1+\alpha)(1+\delta\alpha)Z - (1-\alpha)(1-\delta\alpha)]$,
- Lorentz B_ED: $[(1+\delta+\omega\eta_{\mathrm{s}})Z^2 - 2Z + (1-\delta+\omega\eta_{\mathrm{s}})]$,
- Lorentz B_EPJ: $[(1+\delta+\frac{1}{2}\omega\eta_{\mathrm{s}})Z^2 - (2-\omega\eta_{\mathrm{s}})Z + (1-\delta+\frac{1}{2}\omega\eta_{\mathrm{s}})]$,
- Lorentz BJ_EP: $[(1+\delta)Z^2 - 2(1-\omega\eta_{\mathrm{s}})Z + (1-\delta)]$.

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 occurs only for the Lorentz B_ED scheme when $\varepsilon_{\mathrm{s}} = \varepsilon_\infty$, and $q = 2\omega/(1+\omega)$, which is a resonant value we have already pointed out in the undamped case for this scheme.

In the three-dimensional context, the characteristic polynomial reads

$$\phi_0^{3D}(Z) = [Z-1]^2\psi_0(Z)\left(\phi_0^{1D}(Z)\right)^2$$

for all the schemes we have studied. In addition to extra eigenvalues 1, we have to check cases when we found out that $\phi_0^{1D}(Z)$ is a von Neumann polynomial but not a

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Schur polynomial. If $\varepsilon_s = \varepsilon_\infty$, then we systematically have instabilities. Other extra instable cases depend on the scheme: $q = 4$ for the Debye B_ED and B_EP schemes, $\delta = 1$ for the Debye BP_E scheme; $q = 2$ for the Lorentz D_ED and BJ_EP schemes, $\nu = 0$ for all Lorentz schemes.

We do not have any explanation for these factorizations. This is a property of the characteristic polynomial and not necessarily of the amplification matrix, i.e., this may occur even if variables are not decoupled. However, there is probably some underlying block-triangular structure, which is still to be found.

We shall not duplicate Tables 3.3 and 4.4 for two- and three-dimensional schemes. In the two-dimensional case, if $h_x = h_y = h_z \equiv h$, condition $q \leq 4$ becomes $k \leq h/(\sqrt{2}c_\infty)$ and condition $q \leq 2$ becomes $k \leq h/(2c_\infty)$ in the physical variables. Besides, the Lorentz B_ED model, which was leading to a lower bound on $h$ in the undamped case, leads also to such a bound in the damped case. These are the only differences with Tables 3.3 and 4.4.

In short, three-dimensional conditions are also essentially the same as one-dimensional conditions but inequalities always have to be strict and limiting (nonphysical) cases $\varepsilon_s = \varepsilon_\infty$ and $\nu = 0$ cannot be dealt with properly with a three-dimensional model.

**7. 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 [10] who performs the same analysis but uses specific values for the physical and numerical constants, and uses numeric routines to locate eigenvalues of the amplification matrix. Here we have general results which yield 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 condition as the Yee scheme for nanosecond delay materials. The B_ED and B_EP schemes overcome the BP_E scheme in terms of stability condition for picosecond delay materials. Among the studied schemes for Lorentz media, the B_EPJ scheme clearly ranks first as far as stability is concerned. Its stability condition is also that of the Yee scheme. However, to properly take into account the Lorentz model, a smaller time step may have to be chosen, independently of stability issues. The two examples do not help us to deduce a general strategy to locate variables in time, in order to treat other physical models.

The computer algebra system that has been developed to handle the three-dimensional schemes has a much wider range of application. First, it can be extended with very small effort to other electromagnetic linear models such as cold plasmas, collisionless warm plasmas, or magnetic ferrites. With some more work (no computation skill but knowledge of dimensionless variables), it can be practically extended to the analysis of any linear finite-difference scheme occurring in areas other than electromagnetism.

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