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Von-Neumann stability analysis of FD–TD methods in complex media

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***Abstract* — The stability analysis of Finite Difference–Time Difference (FD–TD) schemes can be reduced *via* the von Neumann approach to the study of a sequence of polynomials with coefficients depending on the physical parameters of the medium and the numerical parameters. Such computations are very tedious in 3D since the simplest medium involves 9th degree polynomials. A Computer Algebra environment has been designed to automize such calculations. This technique is demonstrated on schemes for Maxwell–Debye and Maxwell–Lorentz systems.**

I. INTRODUCTION

The numerical simulation of the propagation of an electromagnetic wave through a dispersive medium can be performed with various techniques, as finite differences, finite elements, finite volumes, spectral methods, ... We focus here on finite difference–time domain (FD–TD) approaches and their stability analysis. Examples of such coupled systems and associated FD–TD schemes are given in [10] in various physical contexts such as non dispersive anisotropic media, cold plasmas, magneto-ionic media, isotropic collisionless warm plasmas, Debye dielectrics, Lorentz dielectrics, magnetic ferrites. All these media share the characteristic to be described by linear models.

In this paper, examples and results are given for FD–TD discretizations of systems coupling Maxwell equations

$$\partial_t B = -\mathrm{curl} E, \tag{1}$$
$$\partial_t D = \mathrm{curl} B/\mu_0, \tag{2}$$

where μ_0 is the vacuum permeability, with Debye equation

$$t_r \partial_t D + D = t_r \varepsilon_0 \varepsilon_\infty \partial_t E + \varepsilon_0 \varepsilon_s E, \tag{3}$$

where t_r is the relaxation time, ε_0 is the vacuum permittivity, ε_∞ is the infinite frequency relative permittivity and ε_s the static relative permittivity; or with Lorentz equation

$$\partial_t^2 D + \nu \partial_t D + \omega_1^2 D = \varepsilon_0 \varepsilon_\infty \partial_t^2 E + \nu \varepsilon_0 \varepsilon_\infty \partial_t E + \varepsilon_0 \varepsilon_s \omega_1^2 E, \tag{4}$$

where in addition ν is damping coefficient and ω_1 the resonance frequency. For such models it is customary to use the electric and magnetic fields $E(x,t)$ and $B(x,t)$ as variables in Maxwell equations. The use of the electric displacement $D(x,t)$ is only here as an example and some schemes are derived using the polarization vector $P(x,t)$ ($D = \varepsilon_0 \varepsilon_\infty E + P$) or the electric current density $J(x,t)$ ($J = \partial_t P$). The various schemes we cite below use these different formulations.

A well known result (Lax–Richtmyer theorem) is that a consistent scheme associated to a well-posed partial differential equation is convergent if and only if it is stable. We will only consider consistent schemes and stability is therefore the only property needed to ensure convergence. As we will describe in Section II this reverts to locate the roots of some polynomial in the unit complex disk. Such an analysis has been already performed by Petropoulos [6] for Maxwell–Debye and Maxwell–Lorentz models, but he used numerical routines to locate the roots once having chosen some specific physical (e.g. relaxation time) and numerical (time and space steps) parameters.

The computation of the roots with given parameters is however not necessary and our goal here is to improve the method in [6] and derive exact (and simple) stability conditions, i.e. possible values of the time step δt in terms of the space step and the physical parameters. The analysis is therefore carried out once and for all for each scheme (and is valid for any value of the parameters), yielding a simple result and allowing to compare the different possible schemes for a same model. Calculations are tedious if one wants to derive the conditions for all the schemes (more than twenty in [10]) and in all dimensions and polarizations. 3D calculations are almost impossible to do by hand without mistaking. We have therefore automated all calculations in a Computer Algebra environment based on MAPLE.

All our schemes derive from Yee scheme [8] for Maxwell equations. This scheme uses staggered grids in space and time. In 1D, given uniform time and space steps δt and δx, variables $E(x,t)$ and $D(x,t)$ are discretized at time–space points $(j\delta x, n\delta t)$ by E_j^n and D_j^n, while $B(x,t)$ is discretized at points $((j+1/2)\delta x, (n-1/2)\delta t)$ by $B_{j+1/2}^{n-1/2}$. Faraday and Ampère equations (1)–(2) are then discretized by

$$\frac{B_{j+1/2}^{n+1/2} - B_{j+1/2}^{n-1/2}}{\delta t} + \frac{E_{j+1}^n - E_j^n}{\delta x} = 0, \tag{5}$$
$$\frac{D_j^{n+1} - D_j^n}{\delta t} + \frac{1}{\mu_0} \frac{B_{j+1/2}^{n+1/2} - B_{j-1/2}^{n+1/2}}{\delta x} = 0. \tag{6}$$

If $D = \varepsilon_0 \varepsilon_\infty E$ (pure Maxwell equations) the stability condition is $\delta t \leq \delta x / c_\infty$, where $\varepsilon_0 \varepsilon_\infty \mu_0 c_\infty^2 = 1$. If variables P or J used instead of D, they can also be taken at integer or half-integer times. This yields for the same physical model a large class of possible schemes.

In Section II, we describe briefly the principle of von Neumann stability analysis. Section III is devoted to the treatment of a simple 1D example. Other schemes are cited in Section IV with the associated stability results. In Section V, we finally describe the principles that led us for the definition of an adapted Computer Algebra environment.

II. PRINCIPLE OF THE STABILITY ANALYSIS

A. Stability

Since we only deal with linear models, we can analyze them in the frequency domain. Thus we assume that the scheme handles a single (vector valued) variable U_j^n with spatial dependence $U_j^n = U^n \exp(i\xi j)$. The scheme is then described as $U^{n+1} = GU^n$ and in our case the amplification matrix G does not depend on time or on δx and δt separately but

only on the ratio $\delta x/\delta t$. This ensures that $U^n = G^n U^0$ and stability comes to the boundedness of G^n. A necessary stability condition is that the eigenvalues of G lie in the unit disk. Only eigenvalues on the unit circle can cause instabilities and two cases can occur:
(a) the eigenvalues of modulus 1 are simple and the scheme is stable. Stability analysis is performed on the characteristic polynomial of G using the tools described in Section II.B;
(b) some eigenvalues of modulus 1 are multiple and stability is obtained if and only if the associated minimal subspaces are of dimension 1. The analysis of the characteristic polynomial does not yield any information on the associated subspaces. Matrix G has to be studied. In our study, this corresponds to degenerate cases for which matrix G has always a very specific form and minimal subspaces are easy to determine. A toy case to illustrate this are the following matrices (which share the same characteristic polynomial):

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

which is typical of the stable case (1 is a double eigenvalue and minimal stable subspaces are 1-dimensional) and

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

which shows an unstable (sometimes called weakly unstable) case (1 is a double eigenvalue and the minimal stable subspace is 2-dimensional).

B. Von Neumann analysis

To prove case (a) above, we study the characteristic polynomial ϕ_0 of G. Its roots are the eigenvalues of G. 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: von Neumann analysis (which is detailed in e.g. [7]) consists in constructing finite sequences of polynomials with decreasing degree which preserve the property to be Schur polynomials or simple von Neumann polynomials, which are defined as follows: a Schur polynomial has all its roots r inside the unit circle ($|r| < 1$); a simple von Neumann polynomial has all its roots r in the unit circle ($|r| \leq 1$), and roots on the unit circle are simple.

Let ϕ 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 ϕ^* by $\phi^*(z) = c_p^* + c_{p-1}^* z + \cdots + c_0^* z^p$. Given a polynomial ϕ_0, we can define a sequence of polynomials

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

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 (i) ϕ_{m+1} is a simple von Neumann polynomial and $|\phi_m(0)| \leq |\phi_m^*(0)|$, or (ii) ϕ_{m+1} is identically zero and ϕ_m' is a Schur polynomial.*

To analyze ϕ_m, 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 0.

III. AN EXAMPLE

We give briefly the outline of the proof for one specific scheme due to Joseph et al. [3] for a Debye medium in 1D : Equations (5) and (6) are supplemented with

$$t_r \varepsilon_0 \varepsilon_\infty \frac{E_j^{n+1} - E_j^n}{\delta t} + \varepsilon_0 \varepsilon_s \frac{E_j^{n+1} + E_j^n}{2} = t_r \frac{D_j^{n+1} - D_j^n}{\delta t} + \frac{D_j^{n+1} + D_j^n}{2}. \quad (7)$$

Equation (7) is the discrete equivalent to the Debye law (3).

Here $U_j^n = {}^t(c_\infty B_{j+1/2}^{n-1/2}, E_j^n, D_j^n/\varepsilon_0\varepsilon_\infty)$ and the amplification matrix is

$$G = \begin{pmatrix} 1 & -\sigma & 0 \\ \frac{(1+\delta)\sigma^*}{1+\delta\eta_s} & \frac{(1-\delta\eta_s)-(1+\delta)\sigma\sigma^*}{1+\delta\eta_s} & \frac{2\delta}{1+\delta\eta_s} \\ \sigma^* & -\sigma\sigma^* & 1 \end{pmatrix}$$

where $\lambda = \delta t/\sqrt{\varepsilon_0\varepsilon_\infty\mu_0}\delta x$, $\delta = \delta t/2t_r$, $\eta_s = \varepsilon_s/\varepsilon_\infty$ and $\sigma = \lambda(e^{i\xi} - 1)$ are dimensionless parameters.

The associated characteristic polynomial ϕ_0 does not depend on σ but only on $q \equiv \sigma\sigma^* = 4\lambda^2 \sin^2(\xi/2)$ (this is a generic situation, not specific to this scheme). It reads

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

We also compute

$$\begin{aligned} \phi_1(Z) &= 2\delta\{2\eta_s Z^2 - [4\eta_s - (\eta_s+1)q]Z \\ &\quad +[2\eta_s - (\eta_s-1)q]\}, \\ \phi_2(Z) &= 4\delta(\eta_s-1)q\{[4\eta_s-(\eta_s-1)q]Z \\ &\quad -[4\eta_s-(\eta_s+1)q]\}. \end{aligned}$$

Parameter δ cannot vanish but we detect at once that a separate study has to be performed for $\eta_s = 1$ and $q = 0$. The case $\eta_s = 1$ is not physical since taking $\varepsilon_s = \varepsilon_\infty$ decouples the system. It is however interesting to know how the scheme behaves in this limiting case. The case $q = 0$ has absolutely to be handled since $q = 0$ if $\xi = 0[\pi]$ and stability has to be proved for all $\xi \in \mathbb{R}$.

We do not expect a better result than for the pure Maxwell case and restrict our study to $q \in [0, 4]$. For Eqs. (5–7), a general case is found, where $q \in (0, 4)$ and $\eta_s > 1$ and we conclude that ϕ_0 is a Schur polynomial. Simple or double roots on the unit circle occur in the other cases but lead to an unbounded G^n sequence only in the case $q = 4$ and $\eta_s = 1$. The different sub-cases and their treatment are summarized in Table I. The main conclusion is that if $\eta_s > 1$, stability is ensured if and only if $q \leq 4$, i.e. $\delta t \leq \delta x/c_\infty$ in dimensional variables.

IV. OTHER SCHEMES FOR MAXWELL–DEBYE AND MAXWELL-LORENTZ EQUATIONS — RESULTS

One of the characteristics of Yee scheme and its coupling with e.g. (7) is to be order two. We do not prove this here but this is due to the space and time centering of the discretization of all terms in the equations. The possible centered formulations are directly linked to the time at which variables are discretized. To automate the process, we had to classify these choices and (5)–(7) is in our language a "B_ED" scheme, which means that B, E and D are chosen as variables, B being discretized at half time steps, E and D at integer time steps.

Below, schemes are only described and stability results given. The detailed 1D analysis can be found in [1, 2].

TABLE I. SPECIFIC CASES FOR THE VON NEUMANN STABILITY ANALYSIS OF EQUATIONS (6)–(7)

Case	Method and result
$q \in (0,4)$, $\eta_s > 1$	Theorem 1 $\Rightarrow$ stable
$q \in (0,4)$, $\eta_s = 1$	Theorem 2 $\Rightarrow$ stable
$q = 0$, $\eta_s \geq 1$	Analysis on G Minimal subspaces of dimension 1 $\Rightarrow$ stable
$q = 4$, $\eta_s > 1$	Theorem 2 $\Rightarrow$ stable
$q = 4$, $\eta_s = 1$	Analysis on G Minimal subspace of dimension 2 $\Rightarrow$ **unstable**

A. *Debye media*

We have dealt with two other schemes than (7) for Debye media. In [9], Young derives a "BP_E" scheme:

$$t_r \frac{P_j^{n+1/2} - P_j^{n-1/2}}{\delta t} = -\frac{P_j^{n+1/2} + P_j^{n-1/2}}{2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty) E_j^n,$$

$$t_r J_j^{n+1/2} = -P_j^{n+1/2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\frac{E_j^{n+1} + E_j^n}{2}.$$

In some sense Debye equation is discretized twice. This is coupled with a "BJ_E" equivalent of Equation (6) and variable J is then cancelled, which avoids redundancy.
In [4], Kashiwa et al. derive a "B_EP" scheme:

$$t_r \frac{P_j^{n+1} - P_j^n}{\delta t} = -\frac{P_j^{n+1} + P_j^n}{2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\frac{E_j^{n+1} + E_j^n}{2},$$

which has to be coupled with a "B_EP" equivalent of Equation (6).

We have to notice that the "BP_E" and "B_PE" schemes lead to the same characteristic polynomial. With the same proof outline as in Section III, we obtain results displayed in Table II in dimensional variables and for $\eta_s > 1$.

TABLE II. 1D STABILITY CONDITIONS FOR DEBYE MEDIA

Scheme	1D stability condition
Joseph et al.	$\delta t \leq \delta x / c_\infty$
Young	$\delta t \leq \min(\delta x / c_\infty, 2t_r)$
Kashiwa et al.	$\delta t \leq \min(\delta x / c_\infty, 2t_r)$

Results in 2D and 3D are essentially the same. To compare schemes we have to compare $2t_r$ and $\delta x / c_\infty$ in realistic contexts. Debye laws are usually valid with centimetric waves, which roughly corresponds to $\delta x / c_\infty \lesssim 10^{-11}$s. This exactly the order of $2t_r$ for water [11]. The choice of the scheme is therefore an important issue for water. But, for a 0.25-dB loaded foam [5], $2t_r \simeq 10^{-9}$s and all the schemes are equivalent from the stability point of view.

B. *Lorentz media*

For Lorentz media you can find "B_ED", "BJ_EP" and "B_EPJ" in [3], [9] and [4] respectively.

• Joseph et al. scheme

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

is coupled with Equation (6). D_j^{n-1} is cancelled from the equations because of redundancy, but E_j^{n-1} is kept. In some sense it is a "B_EED" scheme and there are four variables in 1D as for the following schemes.

• Young scheme

$$\frac{J_j^{n+1/2} - J_j^{n-1/2}}{\delta t} = -\nu \frac{J_j^{n+1/2} + J_j^{n-1/2}}{2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2 E_j^n - \omega_1^2 P_j^n,$$

$$\frac{P_j^{n+1} - P_j^n}{\delta t} = J_n^{n+1/2}$$

has to be coupled with a "BJ_E" version of Equation (6) but this time no redundancy is induced by the choice of variables.

• Kashiwa et al. scheme

$$\frac{J_j^{n+1} - J_j^n}{\delta t} = -\nu \frac{J_j^{n+1} + J_j^n}{2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2 \frac{E_j^{n+1} + E_j^n}{2} - \omega_1^2 \frac{P_j^{n+1} + P_j^n}{2},$$

$$\frac{P_j^{n+1} - P_j^n}{\delta t} = \frac{J_j^{n+1} + J_j^n}{2}$$

has to be coupled with a "B_EP" version of Equation (6).

Once more we apply the von Neumann analysis to obtain the results displayed in Table III in dimensional variables, for $\eta_s > 1$ and $\nu > 0$.

TABLE III. 1D STABILITY CONDITIONS FOR LORENTZ MEDIA

Scheme	1D stability condition
Joseph et al.	$\delta t \leq \delta x / \sqrt{2} c_\infty$
Young	$\delta t \leq \min(\delta x / \sqrt{2} c_\infty, 2/\omega_1 \sqrt{2\eta_s - 1})$
Kashiwa et al.	$\delta t \leq \delta x / c_\infty$

Similar results are valid for multidimensional equations or media with multiple resonant frequencies. The typical wave range for the Lorentz model is micrometric waves. However very different media can be found in the literature. In [6], $\varepsilon_\infty = 1$, $\varepsilon_s = 2.25$ and $\omega_1 = 4\ 10^{16}$rad s^{-1}. In this case $\delta t \leq 2/\omega_1\sqrt{2\eta_s - 1}$ is a very restrictive condition which rules out Young scheme. A totally different material is used in [9] with $\varepsilon_\infty = 1.5$, $\varepsilon_s = 3$ and $\omega_1 = 2\pi\ 5\ \ 10^{10}$rad s^{-1}. Then $\delta t \leq 2/\omega_1\sqrt{2\eta_s - 1}$ is a weak condition compared to $\delta t \leq \delta x / c_\infty$ and any of the three schemes can be used, with a slight advance for Kashiwa et al. scheme, as far as stability is concerned.

V. AUTOMATION *VIA* A COMPUTER ALGEBRA ENVIRONMENT

For a 3D Lorentz medium, ϕ_0 is typically a 12th degree polynomial with polynomial coefficients of degree 6 in the different parameters. The above procedure becomes awful if made by hand. In the cases we treated, the 3D polynomials can be divided twice by the corresponding 1D polynomials and the remaining roots are easy to study. This makes the study easier but you have to able to compute the 3D polynomial to have a chance to notice this.

A Computer Algebra environment based on MAPLE has been developed with the specific aim to automate all the computational steps which may be source of errors. A sample of programme using this environment is given below.

The schemes are defined by four parameters: 1- the space dimension (1, 2 or 3), 2- the polarization (TE or TM in dimension 2), 3- the physical model (e.g. Debye) and 4- the variables used (e.g. `B_ED`).

Maxwell equations have been written once and for all and have just to be "called". For our applications, in the other equations space is only a parameter. Such equations are written once with no spatial dependence and propagated to all the useful coordinates with the right indexes on the staggered grid, according to the space dimension and polarization.

Then change 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 ϕ_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 point from the computer algebra point of view. It comes to evaluate the sign of a polynomial in many variables (4 for a Lorentz medium) and of total degree of order say 6 for ϕ_0, about 10 for ϕ_1, ... knowing some variables are positive (like $\eta_s - 1$ or δ) and other lie within an interval (like q). This is also automated 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 dimension of minimal subspaces and the multiplicity of eigenvalues in the degenerate cases.

```
with(linalg);
read Maxwell; read ChVar;
read vonNeumann;
Dim := 1; Polar := "";
Formula := "B_EP"; Model := "MD";
Eq[1] := Faraday1D;
Eq[2] := Ampere1D_BEP;
Eq[3] := tau*(P[n+1]-P[n])/dt+1/2*P[n+1]
-1/2*eps0*(epss-epsinfty)*(E[n+1]+E[n]);
nbeq := 3;
Var := CalcVar(Dim,Polar,Formula,Model);
G := Amplif(Eq, nbeq, Var);
phi[0] := Ampli2Poly(G, Z);
vonNeumann(phi, Z, nbeq);
fact := Facteurs(phi, Z, nbeq);
rest := Restes(phi, facts, Z, nbeq);
SignCheck(phi, Z, nbeq, [0 < delta, 1 < etas, 0 < q, q < 4]);
```

VI. CONCLUSION

We have developed, and tested on schemes for Maxwell–Debye and Maxwell–Lorentz equations, an efficient way to study the stability of Yee based FD–TD numerical schemes. A Computer Algebra environment makes this procedure tractable for 3D schemes. Some of these scheme have the same stability condition as for the Yee scheme for pure Maxwell equations, but some other schemes do not and we find more restrictive conditions on the time step, which have to be taken into account for certain materials.

Possible developments of this study needing modifications or enlargements of our Computer Algebra environment, but not too much work are (a) non Yee-based schemes, (b) other physical contexts, e.g. collisionless warm plasmas. The same type of toolbox can also be written for fluid dynamics, for example. The key point is that the model is linear or linearized. The von Neumann analysis tools do not have to be modified. Some more work is needed to enlarge the library of classical FD–TD discretizations for the new equations and to define changes of variables which lead to dimensionless variables. This requires a good knowledge of the specific application but no skill in computation by hand.

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