Von-Neumann Stability Analysis of FD–TD methods in complex media

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Outline

1 Motivation
   - Complex optical materials
   - Finite difference schemes and stability

2 Towards an automation of the stability analysis
   - Mathematical tools
   - Computations by hand
   - Automation
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Light propagation is described by Maxwell equations

\[
\begin{align*}
\text{curl } \mathbf{E} & = -\frac{\partial \mathbf{B}}{\partial t} - \mathbf{M}, \\
\text{curl } \mathbf{H} & = \frac{\partial \mathbf{D}}{\partial t} + \mathbf{J},
\end{align*}
\]

\[
\begin{align*}
\text{div } \mathbf{D} & = 0, \\
\text{div } \mathbf{B} & = 0.
\end{align*}
\]

Material properties are described by the constitution laws of the material

\[
\begin{align*}
\mathbf{D} & = \mathbf{D}(\mathbf{E}, \mathbf{H}), \\
\mathbf{B} & = \mathbf{B}(\mathbf{E}, \mathbf{H}), \\
\mathbf{J} & = \mathbf{J}(\mathbf{E}, \mathbf{H}), \\
\mathbf{M} & = \mathbf{M}(\mathbf{E}, \mathbf{H}).
\end{align*}
\]
Material description

- Simple materials: \( D = \varepsilon E \), \( B = \mu H \), \( J = \sigma E \) et \( M = 0 \).

- Examples of complex (linear) materials:
  - anisotropic materials: \( \varepsilon \), \( \mu \) and \( \sigma \) are tensors.
  - cold plasmas, collision-less warm plasmas, magneto-ionic media, magnetic ferrites.

- Debye and Lorentz dielectrics

\[
B = \mu_0 H, \quad M = 0, \quad J = \frac{\partial P}{\partial t} \quad \text{et} \quad D = \varepsilon_0 \varepsilon_\infty E + P.
\]

- Debye: \( \tau \frac{\partial P}{\partial t} + P = \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) E \).

- Lorentz: \( \frac{\partial^2 P}{\partial t^2} + \nu \frac{\partial P}{\partial t} + \omega_1^2 P = \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) \omega_1^2 E \).
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Finite difference schemes

To have explicit and 2-order schemes, models are based on Yee scheme

\[
\frac{B_{j+1/2}^{n+1/2} - B_{j+1/2}^{n-1/2}}{\delta t} = -\frac{E_{j+1}^n - E_j^n}{\delta x},
\]

\[
\varepsilon_0\varepsilon_\infty \frac{E_j^{n+1} - E_j^n}{\delta t} = -\frac{B_{j+1/2}^{n+1/2} - B_{j-1/2}^{n+1/2}}{\mu_0 \delta x} - J_j^{n+1/2},
\]

together with a scheme for matter equations (here Debye–Young)

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

\[
\tau J_j^{n+1/2} = -P_j^{n+1/2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\frac{E_j^{n+1} + E_j^n}{2}.
\]
Former results

Definition of FD–TD schemes
  Yee (1966);
  Luebbers, Hunsberger, Kunz, Standler, Schneider (1990);
  Kashiwa, Yoshida, Fukai (1990);
  Joseph, Hagness, Taflove (1991);
  Luebbers, Steich, Kunz (1993);
  Young (1995);
  Young, Kittichartphayak, Kwok, Sullivan (1995)

Other types of schemes
  Feise, Schneider, Bevelaqua (2004, pseudo-spectral);
  Stoykov, Kuiken, Lowery, Tavlove (2003, FE);

Scheme analysis
  Petropoulos (1994);
  Young (2000)
Aim of the study

Motivations  Petropoulos performs a stability analysis:

1. Explicit form, amplification matrix computation,
2. Characteristic polynomial computation,
3. Choice of physical ($\varepsilon_\infty$, ...) and numerical ($\delta t$, $\delta x$) parameters,

A closed subject? Young “analyzes” the stability of all the above-mentioned schemes using two types of “methods”:

- “the entries for [...] have not been rigorously established”
- “the entry for [...] follows directly from the semi-implicit nature of the scheme”

  false,
  - not really implicit, but written with symmetries.
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Schur and von Neumann polynomials

**Definition**

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

**Definition**

A polynomial is a **von Neumann polynomial** if all its roots $r$ satisfy $|r| \leq 1$.

**Definition**

A polynomial is a **simple von Neumann polynomial** if it is a von Neumann polynomial and its roots of modulus 1 are simple.
Von Neumann analysis

**Theorem**

A *necessary* stability condition is that the characteristic polynomial is a *von Neumann* polynomial.

**Theorem**

A *sufficient* stability condition is that the characteristic polynomial is a *simple von Neumann* polynomial.

Intermediate cases have to be dealt specifically coming back to the structure of the amplification matrix.

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

stable

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

unstable
**Definition**

Let \( \phi(z) = c_0 + c_1 z + \cdots + c_p z^p \) be a polynomial of degree \( p \) with complex coefficients. Its **conjugate polynomial** is

\[ \phi^*(z) = c^*_p + c^*_{p-1} z + \cdots + c^*_0 z^p. \]

From a polynomial \( \phi_0 \), a (finite) sequence of decreasing degree is constructed via the relation

\[ \phi_{m+1}(z) = \frac{\phi_m(0) \phi_m(z) - \phi_m(0) \phi^*_m(z)}{z}. \]

**Theorem**

A polynomial \( \phi_m \) is a Schur polynomial of exact degree \( d \) **iff** \( \phi_{m+1} \) is a Schur polynomial of exact degree \( d - 1 \) and \( |\phi_m(0)| < |\phi^*_m(0)| \).
Sequences of polynomials, II

**Theorem**

A polynomial $\phi_m$ is a simple von Neumann polynomial iff

- either $\phi_{m+1}$ is a simple von Neumann polynomial and $|\phi_m(0)| < |\phi^*_m(0)|$,
- or $\phi_{m+1}$ is identically zero and $\phi'_m$ is a Schur polynomial.

**Difficult problem** localize roots of polynomial of degree 3 to 20 (according to applications and space dimensions) with coefficients depending on 5 to 10 parameters.

**Many “simpler” problems**

- find vanishing conditions for the leading coefficient,
- verify $|\phi_m(0)| < |\phi^*_m(0)|$. 
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1. Find an explicit and dimensionless formulation

\[ U_j^n = (c_\infty B_{j+1/2}^n, E_j^n, P_j^n / \varepsilon_0 \varepsilon_\infty) = \exp(i \xi j) U^n. \]

\[ \lambda = c_\infty \delta t / \delta x, \quad \delta = \delta t / 2 \tau, \quad \eta_s = \varepsilon_s / \varepsilon_\infty, \quad \sigma = \lambda (e^{i \xi} - 1), \quad q = |\sigma|^2. \]

2. Compute the amplification matrix: \( U^{n+1} = G U^n \)

\[ G = \begin{pmatrix}
1 & -\sigma & 0 \\
(1+\delta)\sigma^* & (1-\delta \eta_s)(1+\delta)q & 2\delta \\
\sigma^* & -q & 1+\delta \eta_s
\end{pmatrix}. \]

3. Compute the characteristic polynomial

\[ P(Z) \propto \phi_0(Z) = [1 + \delta \eta_s] Z^3 - [3 + \delta \eta_s - (1 + \delta)q] Z^2 \\
+ [3 - \delta \eta_s - (1 - \delta)q] Z - [1 - \delta \eta_s]. \]
Sequence of polynomials

\[\phi_1(Z) = 2\delta\{2\eta_s Z^2 - [4\eta_s - (\eta_s + 1)q]Z + [2\eta_s - (\eta_s - 1)q]\},\]

\[\phi_2(Z) = 24\delta^2(\eta_s - 1)q\{[4\eta_s - (\eta_s + 1)q]Z - [4\eta_s - (\eta_s + 1)q]\}.\]

Check \(|\phi_m(0)| < |\phi^*_m(0)|\) and the degree

- \(m = 0\): OK,
- \(m = 1\): \(q \in [0, 4]\) is needed (CFL condition \(\lambda \leq 1\) for Yee scheme in 1D). Equality if \(q = 0\) or \(\eta_s = 1\).
- \(m = 2\): Equality if \(q = 4\).

Specific cases

- \(q = 0\): 1 is a double eigenvalue of \(G\) in two stable vector subspaces.
- \(\eta_s = 1\): \(\phi_1\) has two distinct complex roots if \(q \in ]0, 4[\).
- \(q = 4\) and \(\eta_s \neq 1\): \(\phi_2\) has -1 as only root.
- \(q = 4\) and \(\eta_s = 1\): \(G\) has only one eigendirection associated to the double eigenvalue -1 \(\Rightarrow\) instability!
Conclusion on the computation by hand

Results

- Results in accordance with the partial results of Petropoulos, but not with all those intuitive of Young.
- 1D is tractable by hand.

<table>
<thead>
<tr>
<th>Model</th>
<th>Scheme</th>
<th>CFL (1D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Debye</td>
<td>B_ED</td>
<td>$\delta t \leq \delta x/c_\infty$</td>
</tr>
<tr>
<td></td>
<td>B_EP</td>
<td>$\delta t \leq \min(\delta x/c_\infty, 2\tau)$</td>
</tr>
<tr>
<td></td>
<td>BP_E</td>
<td>$\delta t \leq \min(\delta x/c_\infty, 2\tau)$</td>
</tr>
<tr>
<td>Lorentz</td>
<td>B_ED</td>
<td>$\delta t \leq \delta x/\sqrt{2}c_\infty$</td>
</tr>
<tr>
<td></td>
<td>B_EPJ</td>
<td>$\delta t &lt; \delta x/c_\infty$</td>
</tr>
<tr>
<td></td>
<td>BJ_EP</td>
<td>$\delta t \leq \min(\delta x/\sqrt{2}c_\infty, 2/\omega_1 \sqrt{2\eta_s - 1})$</td>
</tr>
</tbody>
</table>

- 2D is tractable by hand, thanks to the experience of 1D: 1D is a factor of the 2D.
- 3D is not reasonable by hand.
New goals

- Automate computations to grapple the 3D.
- Explain factorizations of polynomials.
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What is automated?

A **Maple** toolbox (collection of routines) has been written. It automates:

- Maxwell equations.
- Matter equations, generalization to 1D, 2D and 3D.
- Suppress redundant equations.
- Dimensionless formulation.
- Explicit formulation.
- Amplification matrix.
- Characteristic polynomial.
- Sequence of polynomials.
- Tests $|\phi_m(0)| < |\phi^*_m(0)|$. 

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**Von Neumann stability analysis**

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What is not (already) automated?

Coupling Maxwell–Debye and Maxwell–Lorentz
- Vanishing leading coefficients.
- and hence : Choice of specific treatments.

Other couplings
- Dimensionless formulation.

Imperfect automation
- Tests $|\phi_m(0)| < |\phi^*_m(0)|$.
  Find the sign of a “high” degree polynomial with a large number of variables, positive ($\eta_s$, $\delta$) or lying in an interval ($q$). According to the run, the result is always true but not necessarily optimal.
# Load toolboxes
restart; with(linalg);
read Maxwell; read ChVar1D; read vonNeumann;

# Definition of the model
Dim := 1; Polar := ""; Formula := "B_EP"; Model := "MD";
Eq[1] := Faraday1D;
Eq[2] := Ampere1D_EBP;
Eq[3] := tau*(P[n+1]-P[n])/dt+1/2*P[n+1]
-1/2*eps0*(epss-epsinfini)*(E[n+1]+E[n]);
nbeq := 3;

# Dimensionless formulation
Var := CalcVar(Dim, Polar, Formula, Model);
# Characteristic polynomial
G := Amplif(Eq, nbeq, Var);
phi[0] := Ampli2Poly(G, Z);
save phi, "MD_1D_BEP.m";
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save phi, "MD_1D_BEP.m";
# Von Neumann Sequence

\[
\text{vonNeumann}(\phi, Z, nbeq);
\]

\[
\text{fact} := \text{facteurs}(\phi, Z, nbeq);
\]

\[
\text{rest} := \text{restes}(\phi, \text{fact}, Z, nbeq);
\]

# Sign study in the general case

# Vanishing if \(\delta=0\), \(q=0\) et \(\etas=1\)

\[
\text{verif}(\phi, Z, nbeq, [0 < \delta, 1 < \etas, 0 < q, q < 4]);
\]

# Specific case: \(\delta = 0\)

\[
\phi_{\delta=0}[0] := \text{eval}(\phi[0], \delta = 0);
\]

\[
\psi_{\delta=0}[0] := \text{diff}(\phi_{\delta=0}[0], Z);
\]

\[
\text{vonNeumann}(\psi_{\delta=0}, Z, nbeq-1);
\]

\[
\text{verif}(\psi_{\delta=0}, Z, nbeq-1, [1 < \etas, 0 < q, q < 4]);
\]

# Specific case: \(q=0\)

\[
\phi_{q=0}[0] := \text{eval}(\phi[0], q = 0);
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\[
\psi_{q=0}[0] := \text{diff}(\phi_{q=0}[1], Z);
\]

\[
\text{verif}(\psi_{q=0}, Z, 1, [0 < \delta, 1 < \etas]);
\]

\[
G_{q=0} := \text{eval}(G, q = 0);
\]
Example: Maxwell–Debye–Young 1D, II

# Von Neumann Sequence
vonNeumann(\phi, Z, nbeq);

# Sign study in the general case
# Vanishing if delta=0, q=0 et etas=1
verif(\phi, Z, nbeq, \{0 < \delta, 1 < \etas, 0 < q, q < 4\});

# Specific case: \delta = 0
phidelta_0[0] := eval(\phi[0], \delta = 0);
psidelta_0[0] := diff(phidelta_0[0], Z);
vonNeumann(psidelta_0, Z, nbeq-1);
verif(psidelta_0, Z, nbeq-1, \{1 < \etas, 0 < q, q < 4\});

# Specific case: q=0
phi_q_0[0] := eval(\phi[0], q = 0);
vonNeumann(phi_q_0, Z, nbeq);
psiq_0[0] := diff(phi_q_0[1], Z);
verif(psiq_0, Z, 1, \{0 < \delta, 1 < \etas\});
Gq_0 := eval(G, q = 0);
Example: Maxwell–Debye–Young 1D, II

# Von Neumann Sequence
vonNeumann(phi, Z, nbeq);

fact := facteurs(phi, Z, nbeq);
rest := restes(phi, facts, Z, nbeq);

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verif(phi, Z, nbeq, [0 < delta, 1 < etas, 0 < q, q < 4]);

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Gq0 := eval(G, q = 0);
# Von Neumann Sequence

```plaintext
tvonNeumann(phi, Z, nbeq);
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rest := restes(phi, facts, Z, nbeq);

# Sign study in the general case
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verif(psiq0, Z, 1, [0 < delta, 1 < etas]);
Gq0 := eval(G, q = 0);
```
Conclusion

- **Stability conditions** for FD–TD schemes for Maxwell–Debye and Maxwell–Lorentz systems.
- **Definition of a general strategy** to analyze the stability of FD–TD schemes.

**Future**
- Explain factorizations.
- Application to other complex models and other fields of applications.
- Distribute the toolbox *via* a web page.
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**Thanks for your attention!**