Schémas en temps pour le couplage des équations de Maxwell dans des milieux matériels complexes

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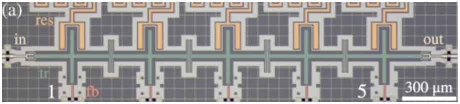
Outline

1. Context – the Anaïs project
2. Models of dispersive materials in optics
3. Numerical schemes
   - Main goals and space and time locations
   - Numerics for Debye media
   - Numerics for Lorentz media
4. Conclusion and perspectives

The Anaïs project

Analyse Numérique et Asymptotique de l'Interaction de Structures photoniques et quantiques via un champ électromagnétique

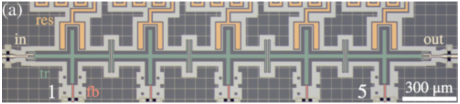
- MITI 80|Prime: project funded by the interdisciplinary mission of the CNRS.
- Collaboration with physicists from the Charles Coulomb Laboratory (Montpellier): Didier Felbacq and Emmanuel Rousseau.



- Underlying dispersive material dispersif with a photonic structure
- Quantum inclusions

Image from Gleb P. Fedorov et al, *Photon transport in a Bose-Hubbard chain of superconducting artificial atoms*, Phys. Rev. Lett. 126(18), 180503 :1–6, 2021.

Goals



- Goal of physists
  - Study the frequency response of the whole device (measure at the output of the device).
  - Modification of the properties of the photonic structure to obtain properties that are not reachable with bulk material (meta-materials).
- Goal of mathematicians
  - Study transient phenomena (and therefore in time).
  - Modification of the properties of the quantum structures by their inclusion in a photonic structure.

Previous works

- Implementation of schemes defined in B. *Stability of FD-TD schemes for Maxwell–Debye and Maxwell–Lorentz equations*, SIAM J. Numer. Anal., **46**, 2251–2566 (2008).
- Inspiration Joly, Vacus, *Mathematical and numerical studies of non linear ferromagnetic materials*, Math. Model. Numer. Anal., **33**, 593–626 (1999).
- Key point: the time localization of variables.
  Method: linear stability analysis studying the eigenvalues of the gain matrix.

LABORATOIRE JEAN KUNTZMANN MATHÉMATIQUES APPLIQUÉES - INFORMATIQUE

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MATHÉMATIQUES APPLIQUÉES - INFORMATIQUE

Maxwell Equations

We consider Maxwell Equations

$$\partial_t \mathsf{B} = -\operatorname{curl} \mathsf{E}, \qquad \text{(Faraday)}$$

$$\partial_t \mathsf{E} = c_\infty^2 \operatorname{curl} \mathsf{B} - \frac{1}{\varepsilon_0 \varepsilon_\infty} \partial_t \mathsf{P}. \qquad \text{(Ampère)}$$

- No magnetization : $\mathsf{B} = \mu_0 \mathsf{H}$.
- Modulo some restrictions on described materials, we can choose dimensions for the space and the fields.
- We will also use $\mathsf{J} = \partial_t \mathsf{P}$ but not $\mathsf{D} = \varepsilon_0 \varepsilon_\infty \mathsf{E} + \mathsf{P}$.

Notations: ε_∞: relative permittivity at infinite frequency, $\varepsilon_0 \varepsilon_\infty \mu_0 c_\infty^2 = 1$.

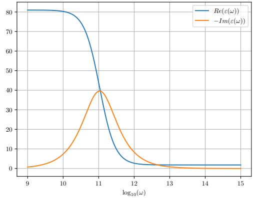
Debye model

The polarisation is solution to a delay equation

$$t_r \partial_t P + P = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)E.$$

This corresponds to the relative frequency

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\varepsilon_s - \varepsilon_\infty}{1 + i\omega t_r}.$$



Water

Notations: ε_s : static (zero frequency) relative permittivity, t_r: delay.

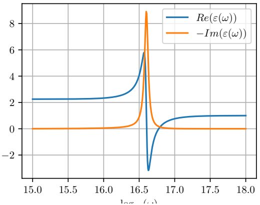
Lorentz model

There is one (possibly many) resonant frequency and the polarisation is solution to

$$\partial_t^2 P + \nu \partial_t P + \omega_1^2 P = \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2 E.$$

This corresponds to the relative frequency

$$\varepsilon_r(\omega) = \varepsilon_\infty + \frac{\omega_1^2(\varepsilon_s - \varepsilon_\infty)}{\omega_1^2 + i\omega\nu - \omega^2}.$$



Notations: ε_s : static (zero frequency) relative permittivity, ν: relaxation rate, ω_1: resonant frequency.

Energy estimates 1/2

Defining the energy

$$\mathcal{E}_\infty = \frac{\varepsilon_0 \varepsilon_\infty}{2} \left(\|\mathsf{E}\|_{L^2}^2 + c_\infty^2 \|\mathsf{B}\|_{L^2}^2 \right),$$

we have

$$\frac{\mathrm{d}\mathcal{E}_\infty}{\mathrm{d}t} = -\int_{\mathbb{R}^n} \mathsf{J} \cdot \mathsf{E} \, \mathrm{d}x,$$

which we will have to evaluate for each material model.

then, we will define an energy which is specific for each dispersive model and determine how it decreases (since it will decrease...).

Of course if $\mathsf{J} \equiv 0$, then $\mathcal{E}_\infty$ is constant.

Energy estimates 2/2

- For Debye

$$\mathcal{E}_{\mathrm{Debye}} = \mathcal{E}_\infty + \frac{1}{2}\frac{1}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\|\mathsf{P}\|^2_{L^2}$$

and

$$\frac{\mathrm{d}\mathcal{E}_{\mathrm{Debye}}}{\mathrm{d}t} = -\frac{t_r}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\|\mathsf{J}\|^2_{L^2}.$$

- For Lorentz

$$\mathcal{E}_{\mathrm{Lorentz}} = \mathcal{E}_\infty + \frac{1}{2}\frac{1}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\left(\|\mathsf{P}\|^2_{L^2} + \frac{1}{\omega_1^2}\|\mathsf{J}\|^2_{L^2})\right)$$

and

$$\frac{\mathrm{d}\mathcal{E}_{\mathrm{Lorentz}}}{\mathrm{d}t} = -\frac{\nu}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2}\|\mathsf{J}\|^2_{L^2}.$$

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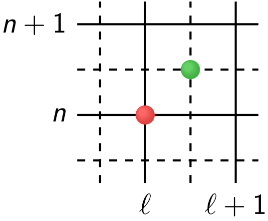
Main goals

- Define schemes for Debye and Lorentz media which are
  - as explicit as possible,
  - preserve physical quantities.
- Possibility to couple with Bloch equations for quantum inclusions
- Space:
  - here finite differences,
  - previously finite volumes,
  - in the future finite elements.

1D Yee scheme

Use of staggered grids

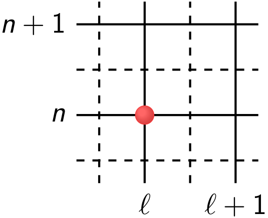


$$\frac{\mathrm{B}_{\ell+\frac12}^{n+\frac12}-\mathrm{B}_{\ell+\frac12}^{n-\frac12}}{\delta t}=-\frac{\mathrm{E}_{\ell+1}^{n}-\mathrm{E}_{\ell}^{n}}{\delta z},$$

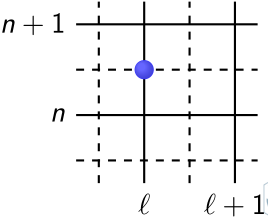
$$\frac{\mathrm{E}_{\ell}^{n+1}-\mathrm{E}_{\ell}^{n}}{\delta t}=-c_\infty^2\frac{\mathrm{B}_{\ell+\frac12}^{n+\frac12}-\mathrm{B}_{\ell-\frac12}^{n+\frac12}}{\delta z}-\frac{1}{\varepsilon_0\varepsilon_\infty}\mathrm{J}_{\ell}^{n+\frac12}.$$

For a new variable

A_ℓ^n



or $\mathrm{A}_\ell^{n+\frac12}$



Discrete energies for a semi-discretization in time

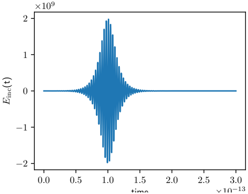
$$\frac{B^{n+\frac{1}{2}} - B^{n-\frac{1}{2}}}{\delta t} = -\operatorname{curl} E^n,$$
$$\frac{E^{n+1} - E^n}{\delta t} = c_\infty^2 \operatorname{curl} B^{n+\frac{1}{2}} - \frac{1}{\varepsilon_0\varepsilon_\infty} J^{n+\frac{1}{2}}.$$

We define $\underline{E}^{n+\frac{1}{2}} = \frac{1}{2}(E^{n+1} + E^n)$ and $\underline{B}^n = \frac{1}{2}(B^{n+\frac{1}{2}} + B^{n-\frac{1}{2}})$ and explore two time centerings for energies (preserved if $J \equiv 0$):

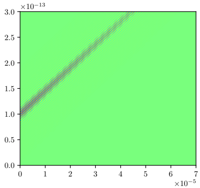
$$\mathcal{E}_\infty^n = \frac{\varepsilon_0\varepsilon_\infty}{2}\left(\|E^n\|^2 + c_\infty^2\|\underline{B}^n\|^2 - \frac{c_\infty^2\delta t^2}{4}\|\operatorname{curl} E^n\|^2\right),$$

$$\mathcal{E}_\infty^{n+\frac{1}{2}} = \frac{\varepsilon_0\varepsilon_\infty}{2}\left(\|\underline{E}^{n+\frac{1}{2}}\|^2 + c_\infty^2\|B^{n+\frac{1}{2}}\|^2 - \frac{\delta t^2}{4}\|\operatorname{curl} B^{n+\frac{1}{2}}\|^2\right).$$

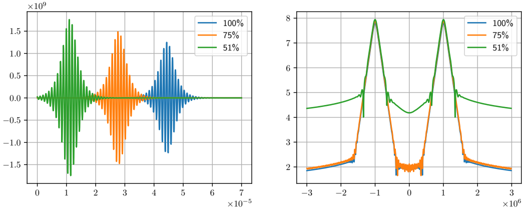
Incident field and result representation



Incident field



Unicorn



E and $\hat{E}$ at different times

Debye B_EP scheme (1/3)

$$\frac{\mathrm{E}^{n+1}-\mathrm{E}^{n}}{\delta t}=c_\infty^2\,\mathrm{curl}\,\mathrm{B}^{n+\frac{1}{2}}-\frac{1}{\varepsilon_0\varepsilon_\infty}\frac{\mathrm{P}^{n+1}-\mathrm{P}^{n}}{\delta t}, \qquad \text{(Ampère)}$$

$$t_r\frac{\mathrm{P}^{n+1}-\mathrm{P}^{n}}{\delta t}=-\frac{\mathrm{P}^{n+1}+\mathrm{P}^{n}}{2}+\varepsilon_0(\varepsilon_s-\varepsilon_\infty)\frac{\mathrm{E}^{n+1}+\mathrm{E}^{n}}{2}. \qquad \text{(Debye)}$$

For $\varepsilon_s > \varepsilon_\infty$, linear stability proved if $c_\infty\delta t/\delta z \leq 1$.

Remark: this is precisely the condition for $\mathcal{E}_\infty^n$ and $\mathcal{E}_\infty^{n+\frac{1}{2}}$ to be positive.

Model from Kashiwa, Yoshida, Fukai, *A treatment by the FD–TD method of the dispersive characteristics associated with orientation polarization*, IEICE Trans., **E73**,1326–1328. (1990).

Debye B_EP scheme (2/3)

We define $\mathcal{E}^n_{\text{Debye B\_EP}}$ as

$$\mathcal{E}^n_{\text{Debye B\_EP}} = \mathcal{E}^n_\infty + \frac{1}{2}\frac{1}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\|\mathsf{P}^n\|^2,$$

and

$$\mathcal{E}^{n+1}_{\text{Debye B\_EP}} = \mathcal{E}^n_{\text{Debye B\_EP}} - \frac{t_r \delta t}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\|\mathsf{J}^{n+\frac{1}{2}}\|^2.$$

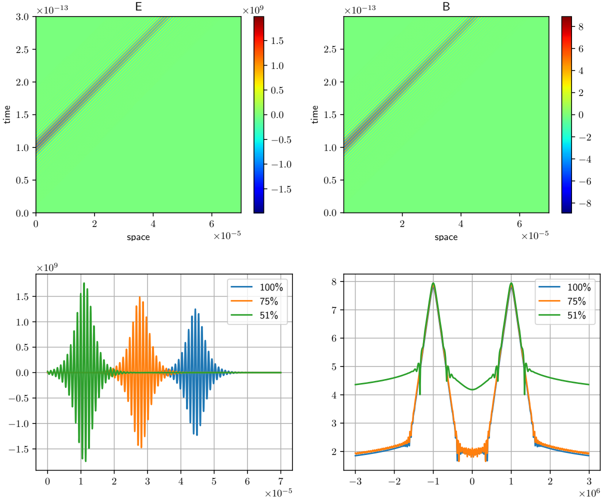
Defining $\mathcal{E}^{n+\frac{1}{2}}_{\text{Debye B\_EP}}$ as

$$\mathcal{E}^{n+\frac{1}{2}}_{\text{Debye B\_EP}} = \mathcal{E}^{n+\frac{1}{2}}_\infty + \frac{1}{2}\frac{1}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\left(\frac{\delta t^2}{4}\|\mathsf{J}^{n+\frac{1}{2}}\|^2 + \frac{\|\mathsf{P}^{n+1}\|^2 + \|\mathsf{P}^n\|^2}{2}\right),$$

we have

$$\mathcal{E}^{n+\frac{1}{2}}_{\text{Debye B\_EP}} = \mathcal{E}^{n-\frac{1}{2}}_{\text{Debye B\_EP}} - \frac{t_r \delta t}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}(\|\mathsf{J}^{n+\frac{1}{2}}\|^2 + \|\mathsf{J}^{n-\frac{1}{2}}\|^2).$$

Debye B_EP scheme (3/3)



Debye BP_E scheme

$$\frac{\mathrm{E}^{n+1} - \mathrm{E}^{n}}{\delta t} = c_\infty^2 \operatorname{curl} \mathrm{B}^{n+1/2} - \frac{1}{\varepsilon_0 \varepsilon_\infty} \mathrm{J}^{n+1/2}, \qquad \text{(Ampère)}$$

$$t_r \frac{\mathrm{P}^{n+1/2} - \mathrm{P}^{n-1/2}}{\delta t} = -\frac{\mathrm{P}^{n+1/2} + \mathrm{P}^{n-1/2}}{2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\mathrm{E}^{n}, \qquad \text{(Debye)}$$

$$t_r \mathrm{J}^{n+1/2} = -\mathrm{P}^{n+1/2} + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\frac{\mathrm{E}^{n+1} + \mathrm{E}^{n}}{2}, \qquad \text{(Debye)}$$

For $\varepsilon_s > \varepsilon_\infty$, linear stability proved if $c_\infty \delta t / \delta z \leq 1$ and $\delta t / 2 t_r \leq 1$.

Model from Young, *Propagation in linear dispersive media: Finite difference time–domain methodologies*, IEEE Trans. Antennas Propag., 43, 422–426 (1995).

Debye BJ_EP scheme

$$\frac{\mathbf{E}^{n+1} - \mathbf{E}^{n}}{\delta t} = c_\infty^2 \operatorname{curl} \mathbf{B}^{n+1/2} - \frac{1}{\varepsilon_0 \varepsilon_\infty} \mathbf{J}^{n+1/2}, \qquad \text{(Ampère)}$$

$$\mathbf{J}^{n+\frac{1}{2}} = \frac{\mathbf{P}^{n+1} - \mathbf{P}^{n}}{\delta t},$$

$$t_r \frac{\mathbf{J}^{n+\frac{1}{2}} + \mathbf{J}^{n-\frac{1}{2}}}{2} = -\mathbf{P}^n + \varepsilon_0(\varepsilon_s - \varepsilon_\infty)\mathbf{E}^n. \qquad \text{(Debye)}$$

Lorentz B_EPJ scheme (1/4)

‘

$$\frac{\mathrm{E}^{n+1}-\mathrm{E}^{n}}{\delta t} = c_\infty^2 \operatorname{curl} \mathrm{B}^{n+1/2} - \frac{1}{\varepsilon_0\varepsilon_\infty}\frac{\mathrm{P}_j^{n+1}-\mathrm{P}_j^{n}}{\delta t}, \qquad \text{(Ampère)}$$

$$\frac{\mathrm{P}^{n+1}-\mathrm{P}^{n}}{\delta t} = \frac{\mathrm{J}^{n+1}+\mathrm{J}^{n}}{2}$$

$$\frac{\mathrm{J}^{n+1}-\mathrm{J}^{n}}{\delta t} = -\nu\frac{\mathrm{J}^{n+1}+\mathrm{J}^{n}}{2} + \omega_1^2\varepsilon_0(\varepsilon_s-\varepsilon_\infty)\frac{\mathrm{E}^{n+1}+\mathrm{E}^{n}}{2} - \omega_1^2\frac{\mathrm{P}^{n+1}+\mathrm{P}^{n}}{2}. \qquad \text{(Lorentz)}$$

For $\varepsilon_s > \varepsilon_\infty$ and $\nu > 0$, linear stability proved if $c_\infty \delta t/\delta z < 1$.

Model from Kashiwa, Yoshida, Fukai, *A treatment by the FD–TD method of the dispersive characteristics associated with orientation polarization*, IEICE Trans., **E73**, 1326–1328 (1990).

Lorentz B_EPJ scheme (2/4)

$$\mathcal{E}^n_{\text{Lorentz B\_EPJ}} = \mathcal{E}^n_\infty + \frac{1}{2\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}\|\mathsf{P}^n\|^2$$

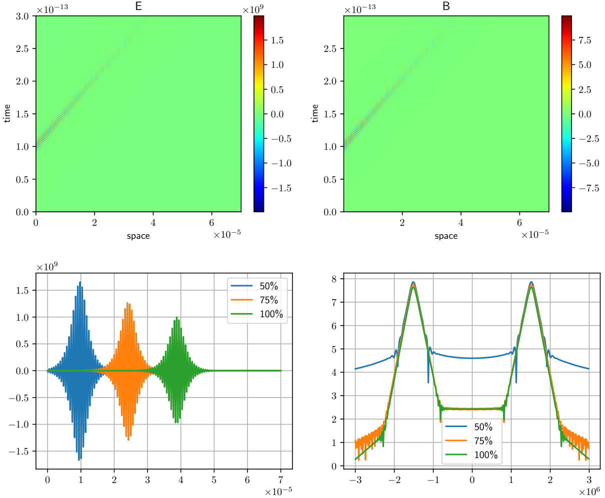
$$\mathcal{E}^{n+1}_{\text{Lorentz B\_EPJ}} = \mathcal{E}^n_{\text{Lorentz B\_EPJ}} - \frac{\nu\delta t}{\varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2}\|\underline{\mathsf{J}}^{n+1/2}\|^2.$$

$$\mathcal{E}^{n+\frac{1}{2}}_{\text{Lorentz B\_EPJ}} = \mathcal{E}^{n+\frac{1}{2}}_\infty + \frac{1}{4\varepsilon_0(\varepsilon_s - \varepsilon_\infty)}(\|\mathsf{P}^{n+1}\|^2 + \|\mathsf{P}^n\|^2) + \frac{1}{4\varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2}(\|\mathsf{J}^{n+1}\|^2 + \|\mathsf{J}^n\|^2)$$

$$\mathcal{E}^{n+\frac{1}{2}}_{\text{Lorentz B\_EPJ}} = \mathcal{E}^{n-\frac{1}{2}}_{\text{Lorentz B\_EPJ}} - \frac{\nu\delta t}{2\varepsilon_0(\varepsilon_s - \varepsilon_\infty)\omega_1^2}(\|\underline{\mathsf{J}}^{n+1/2}\|^2 + \|\underline{\mathsf{J}}^{n-1/2}\|^2).$$

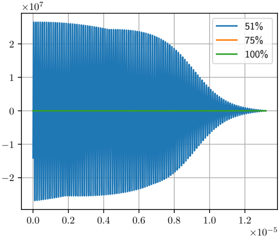
Lorentz B_EPJ scheme (3/4)

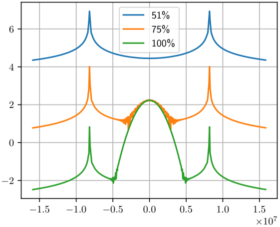
Center frequency: $1.8\ 10^{15}$ Hz



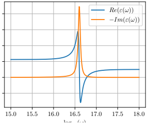
Lorentz B_EPJ scheme (4/4)

Center frequency: 10^{16} Hz





Clearly, as expected, the model is quite sensitive to the input frequency.

Recall: 

Lorentz BJ_EP scheme

$$\frac{E^{n+1} - E^n}{\delta t} = c_\infty^2 \operatorname{curl} B^{n+1/2} - \frac{1}{\varepsilon_0 \varepsilon_\infty} J^{n+1/2}, \qquad \text{(Ampère)}$$

$$\frac{P^{n+1} - P^n}{\delta t} = J^{n+1/2},$$

$$\frac{J^{n+1/2} - J^{n-1/2}}{\delta t} = -\nu \frac{J^{n+1/2} + J^{n-1/2}}{2} + \omega_1^2 \varepsilon_0 (\varepsilon_s - \varepsilon_\infty) E^n - \omega_1^2 P^n, \qquad \text{(Lorentz)}$$

For $\varepsilon_s > \varepsilon_\infty$ and $\nu > 0$, linear stability proved if $c_\infty \delta t / \delta z < \frac{1}{2}$ and $\omega_1^2 \delta t^2 \leq 4/(2\frac{\varepsilon_s}{\varepsilon_\infty} - 1)$.

Model from Young, *Propagation in linear dispersive media: Finite difference time–domain methodologies*, IEEE Trans. Antennas Propag., 43, 422–426 (1995).

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Conclusion and perspectives

- This is a small step towards the main goal.
- Local implicitness is welcome.

- The Bloch equation (governing quantum inclusions) is "known" to have a Lorentz counterpart in certain regimes.
- We expect that having both Bloch and Lorentz will induce a shift in the resonant frequency.
- Possibility to switch the system by acting on the quantum structures.