# Dispersive Materials in Time Domain

## Modelling, Stability and Numerical Results

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# Outline

## Aims

- Model the electric behaviour of arbitrarily dispersive materials starting from a collection of data points.
- Incorporate the model into a Time Domain scheme. In our case, DGTD.

## Faraday's source–free curl equations for dispersive media

$$j\omega\varepsilon\vec{E} = \nabla \times \vec{H}, \quad \varepsilon = \varepsilon(\omega) \tag{1}$$

## Electric Permittivity model

We will use the complex-conjugated pole-residual (CCPR) pairs described in [Han et al., 2006]

$$\varepsilon(\omega) = \varepsilon_0\varepsilon_\infty + \varepsilon_0 \sum_{r=1}^{R} \left[\chi_r(\omega) + \chi_r'(\omega)\right] \tag{2}$$

with

$$\chi_r(\omega) = \frac{c_r}{j\omega - a_r} \quad \text{and} \quad \chi_r'(\omega) = \frac{c_r^*}{j\omega - a_r^*} \tag{3}$$

and $(c_r,\ a_r \in \mathbb{C})$. We also require $\Re\mathrm{e}\{a_r\} < 0$ for stability.

## Polarization currents

In previous model we can identify $\vec{P}_r$ and $\vec{P}'_r$ as polarization currents with,

$$\vec{P}_r = \varepsilon_0 \chi_r \vec{E} \quad \text{and} \quad \vec{P}'_r = \varepsilon_0 \chi'_r \vec{E} \tag{4}$$

In time domain we will always have $\vec{P}'_r = \vec{P}^*_r$, because $\vec{E} \in \mathbb{R}^3$

## CCPR Faraday's Law in Time Domain

We can pass the previous equations into the time domain obtaining,

$$\varepsilon_0 \varepsilon_\infty \partial_t \vec{E} = \nabla \times \vec{H} - \sum_{r=1}^{R} \left( \partial_t \vec{P}_r + \partial_t \vec{P}^*_r \right) \tag{5}$$

## ADE System of coupled equations

After applying the ADE formalism we can rewrite (5) as a system of coupled PDEs.

$$\partial_t \vec{E} = \frac{1}{\varepsilon_0 \varepsilon_\infty} \left[ \nabla \times \vec{H} - 2 \sum_{r=1}^{R} \Re\mathrm{e}\{\partial_t \vec{P}_r\} \right]$$

$$\partial_t \vec{P}_r = a_r \vec{P}_r + \varepsilon_0 c_r \vec{E} \qquad \forall r = 1, \ldots, R \qquad (6)$$

## Analytically

We can note that some of the most commonly used media are particular cases of the model (2).

1. Poles of a Debye's model are obtained when $c_r = \Delta\varepsilon_r/(2\tau_r)$ and $a_r = -1/\tau_r$.
2. Similarly for Lorentz's media we have $c_r = j\Delta\varepsilon_r\omega_r^2/(2\sqrt{\omega_r^2 - \delta_r^2}\,)$ and $a_r = -\delta_r - j\sqrt{\omega_r^2 - \delta_r^2}$.
3. Conductive media can be modeled adding a pole-residue with $a_0 = 0$ and $c_0 = \sigma/(2\varepsilon_0)$.

## Vector Fitting (VF)

In many situations, simulations need to start from a collection of data points for the permittivity. A common process of converting those points into CCPR pairs is Vector Fitting (VF), described in [Gustavsen and Semlyen, 1999] [Gustavsen, 2006] [Deschrijver et al., 2008].

## Availability

The most used routines to perform VF were written by Gustavsen and are available in:

`http://www.energy.sintef.no/Produkt/VECTFIT/`

He also provides packages to ensure passivity of the model.

## Modification of stability conditions

Inclusion of the ADE terms in equations (6) modifies the stability conditions of the system when time integration is performed by modifying the existing eigenvalues and adding new ones.

## Conductive one-dimensional case

For the conductive case (single pole with $a_r = 0$ and $c_r = \sigma/(2\varepsilon_\infty)$) and one dimension we find the following eigenvalue for numerical frequency.

$$\tilde{\omega} = -\frac{\sigma}{2\varepsilon_\infty} \pm \sqrt{\left(\frac{\sigma}{2\varepsilon_\infty}\right)^2 - \left(\frac{\tilde{k}}{\sqrt{\varepsilon_\infty \mu}}\right)^2} \tag{7}$$

with $\tilde{k}$ being the numerical wavenumber [Alvarez et al., 2012a]. More general cases can be studied, but not always we can find an analytical expression (we can found pseudo–analytical).

## Values of $\tilde{k}$, numerical wavenumber

For FD and DG with centered fluxes spatial discretization $\tilde{k} \in \mathbb{R}$.
For FD $\max|\tilde{k}| = h^{-1}$, for DG with centered fluxes $\max|\tilde{k}| = 4(p+1)^2 h^{-1}$. See [Hesthaven and Warburton, 2007], [Taflove and Hagness, 2005].

## Values of $\tilde{\omega}$, numerical frequency

The values of $\tilde{\omega}$ tell us what is the max $\Delta t$ we can choose to ensure stability.

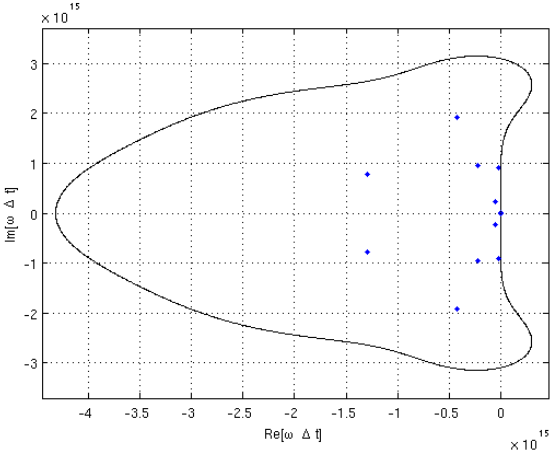
### LF Time integration for a simply conductive material

In the case of LF, the scheme is stable as long as $\Delta t \leq 1/\Im[\tilde{\omega}]$, an open semi–infinite region not limited in $\mathbb{R}$. Therefore, **no value of $\sigma$ will make the scheme unstable**.

### RK Time integration for a simply conductive material

For the RK case the stability region is closed and limited in the $\mathbb{R}$ axis. A value of $\sigma$ big enough will make the scheme unstable. **In other words the $\Delta t$ imposed by $\tilde{k}$ alone could not be sufficient to ensure stability.**

With arbitrary poles ($c_r, a_r \in \mathbb{C}$), **LF and RK can become unstable**. The following figure illustrates the situation for a 5 poles material (modelling silver at THz frequencies) described in [Han et al., 2006].



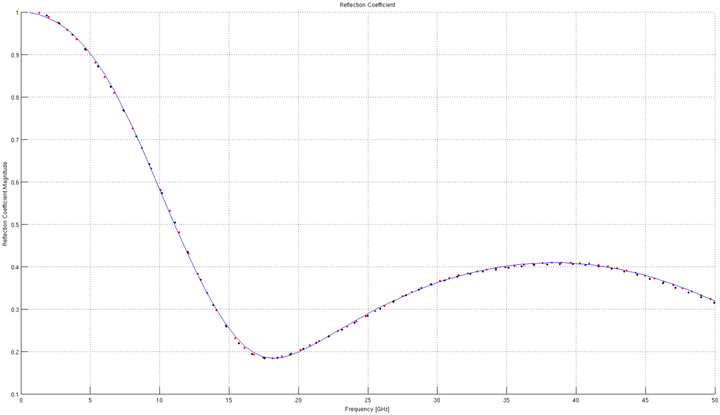
# Possible solution

## Solution at VF stage

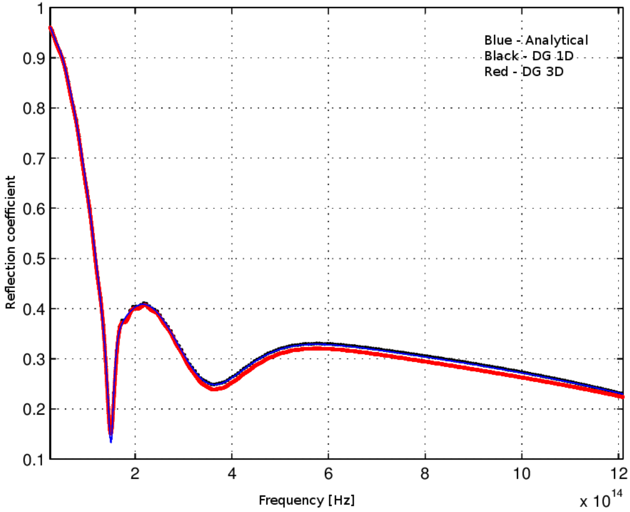
At the VF stage. Ensure that all the poles fall in the stability region. This would require information of the mesh and solver at the vector fitting stage. We have not implemented anything like this yet and what we do is to constrain the poles to have $|a_r|^{-1} < \Delta t$, and pray.

# Results

Reflection coefficient of a PEC backed Debye material, thickness of $0.25mm$, $\varepsilon_\infty = 2$, $\sigma = 2[S/m]$, $(c_1, a_1) = (1/9.4E6, -1/9.4E6)$. Up to $50GHz$. Described in [Garcia et al., 2003]



Silver slab with 5 poles described in [Han et al., 2006]. Thickness of 100$nm$ frequencies up to 1200$THz$.



# Summary

## Arbitrary materials

The method can model any permittivity profile. Classical dispersive models are particular cases. It can start from a collection of data points.

## Stability

Sources of unstability have been detected and analyzed. A solution has been proposed.

## Validity

Results show a good agreement with analytical predictions.

# Still to be done...

## SMA

SMA conditions do not work for truncating dispersive materials. No other absorbing technique has been tested.

## VF feedbacked by solver

An automatic process to generate complex–poles guaranteed to be stable for a given mesh and time integration technique.

## Impedances in fluxes

Fluxes are not included in the ADE formulation. All the impedances are taken at $Z(\omega \to \infty)$. The impact of this approximation should be assesed. It has relevance in anisotropic media [Alvarez et al., 2012b].

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# Thanks. Questions?

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