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Abstract

The numerical study of electromagnetic wave propagation in nanophotonic devices requires among others the integration of various types of dispersion models, such as the Drude one, in numerical methodologies. Appropriate approaches have been extensively developed in the context of the Finite Differences Time-Domain (FDTD) method, such as in [1] for example. For the discontinuous Galerkin time-domain (DGTD), stability and convergence studies have been recently realized for some dispersion models, such as the Debye model [2]. The present study focuses on a DGTD formulation for the solution of Maxwell's equations coupled to (i) a Drude model and (ii) a generalized dispersive model. Stability and convergence have been proved in case (i), and are under study in case (ii). Numerical experiments have been made on classical situations, such as (i) plane wave diffraction by a gold sphere and (ii) plane wave reflection by a silver slab.

1 Drude model

The Drude model describes the response of certain dispersive media to an electromagnetic wave propagating in a certain range of frequencies. The considered model permits to establish a dependency between the permittivity of the material and the angular frequency of the electromagnetic wave in the following form:

$$\varepsilon_{r,d}(\omega) = \varepsilon_\infty - \frac{\omega_d^2}{\omega^2 + i\omega\gamma_d},$$

where ω_d, γ_d and ω are respectively the plasma frequency and the damping constant of the medium, and the angular frequency. Adding a Drude dispersion model therefore implies a coupling, in the time domain, between the electric field $\mathbf{E}$ and an additional field, the dipolar current ($\mathbf{J}_p$), through an ODE whose solution we choose is here approximated in a DG framework. A centered fluxes DG method has been chosen to develop a numerical approximation of the problem, given the geometry and the inhomogeneous media to be considered. It is associated with a second-order Leap-Frog scheme in time, therefore inducing a non-dissipative scheme. A theoretical study of the latter has been made, demonstrating an error convergence in $O\left(h^{\min(s,p)} + \Delta t^2\right)$, where p is the spatial order of approximation, and s is related to the regularity assumptions made on the electromagnetic field.

2 Generalized dispersive model

Recently, several arbitrary dispersive models have been proposed, such as the Critical Points (CP) [3] and the Complex-Conjugate Pole-Residue Pairs (CCPRP) [1]. Here, another formulation is considered: in accordance with the fundamental theorem of algebra, the permittivity function is written as a decomposition of a constant, one zero-order pole (ZOP), a set of first-order generalized poles (FOGP), and a set of second-order generalized poles (SOGP). This leads to the following expression in the frequency domain:

$$\varepsilon_{r,g}(\omega) = \varepsilon_\infty - \frac{\sigma}{j\omega} - \sum_{l\in L_1} \frac{a_l}{j\omega - b_l} - \sum_{l\in L_2} \frac{c_l - j\omega d_l}{\omega^2 - e_l + j\omega f_l}.$$

This general writing allows an important flexibility for two reasons: (i) it unifies most of the common dispersion models in a single formulation (such as Drude, Drude-Lorentz and Debye media for example), and (ii) it permits to fit any experimental data set in a reasonable number of poles (and thus a reasonable number of coefficients). The stability and convergence properties of the resulting DG formulation seem at first glance to be a feasible extension of the Drude case, and are currently under investigation.

3 Numerical validations

First, a simple validation case has been set up in order to verify that the orders of convergence theoretically obtained for the Drude model based DGTD method were achieved. A unitary PEC cavity with dispersive properties defined by a Drude model is defined. A forced source current has been added to the set of equations in order to obtain an analytical solution to compare with. The calculated convergence orders match the theoretical prediction, as presented in table 1.

Then, a more physical case is considered: a gold nanosphere of radius 20 nm, whose properties are described by a Drude model, is illuminated by a plane wave, the latter being modulated in time by a gaussian function. The discrete Fourier transform of the field is processed along the computation, and is in the end compared with the Mie solution[1] of the problem, which is taken as a reference solution. A good adequation has been found between the reference and the numerical solution, which is displayed on figure 1. Further accuracy and performance assessment will be performed on this fondamental case, then paving the way to situations of high interest in the nanophotonic domain.

References

[1] M. Han, R. W. Dutton, and S. Fan. Model dispersive media in FDTD method with complex-conjugate pole-residue pairs. *IEEE Microwave and Wireless Components Letters*, 16:119 – 121, 2006.

[2] Stéphane Lanteri and Claire Scheid. Convergence of a discontinuous Galerkin scheme for the mixed time domain Maxwell's equations in dispersive media. *IMA Journal of Numerical Analysis*, 2012.

[3] A. Vial, T. Laroche, M. Dridi, and L. Le Cunff. A new model of dispersion for metals leading to a more accurate modeling of plasmonic structures using the FDTD method. *Applied Physics A*, 103:849 – 853, 2011.

[1]The Mie theory provides an analytical solution to diffraction problems in the case of spherical obstacles.

Table 1: **Convergence orders with $\mathbb{P}_1$ and $\mathbb{P}_2$ approximations** for the PEC cavity case.

(a) Convergence rate, $\mathbb{P}_1$

Refinement	Convergence rate
$\frac{1}{50}$	–
$\frac{1}{75}$	1.2575
$\frac{1}{100}$	1.1197
$\frac{1}{125}$	1.1000
$\frac{1}{150}$	1.0614

(b) Convergence rate, $\mathbb{P}_2$

Refinement	Convergence rate
$\frac{1}{25}$	–
$\frac{1}{50}$	2.2004
$\frac{1}{75}$	2.0826
$\frac{1}{100}$	2.0366
$\frac{1}{125}$	2.0432

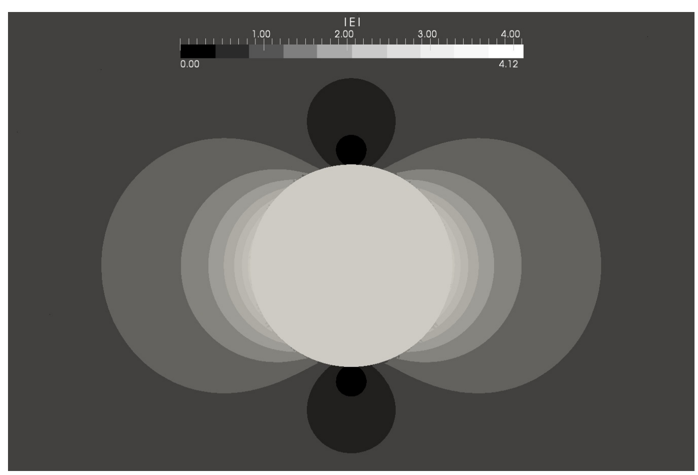

Figure 1: **E field magnitude in the frequency domain calculated by the DGTD method in the vicinity of the gold nanosphere.** The view is a $z = 0$ slice.