

Numerical Modeling of Light/Matter Interaction at the Nanoscale with a High Order Finite Element Type Time-domain Solver

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Abstract— We present a discontinuous finite element (discontinuous Galerkin) time-domain solver for the numerical simulation of the interaction of light with nanometer scale structures. The method relies on a compact stencil high order interpolation of the electromagnetic field components within each cell of an unstructured tetrahedral mesh. This piecewise polynomial numerical approximation is allowed to be discontinuous from one mesh cell to another, and the consistency of the global approximation is obtained thanks to the definition of appropriate numerical traces of the fields on a face shared by two neighboring cells. Time integration is achieved using an explicit scheme and no global mass matrix inversion is required to advance the solution at each time step. Moreover, the resulting time-domain solver is particularly well adapted to parallel computing. The proposed method is an extension of the method that we initially proposed in [1] for the simulation of electromagnetic wave propagation in non-dispersive heterogeneous media at microwave frequencies.

1. INTRODUCTION

The numerical modeling of light interaction with nanometer scale structures generally relies on the solution of the system of time-domain Maxwell equations, possibly taking into account an appropriate physical dispersion model, such as the Drude or Drude-Lorentz models, for characterizing the material properties of metallic nanostructures at optical frequencies [2]. In the computational nanophotonics literature, a large number of studies are devoted to Finite Difference Time-Domain (FDTD) type discretization methods based on Yee's scheme [3]. As a matter of fact, the FDTD [4] method is a widely used approach for solving the systems of partial differential equations modeling nanophotonic applications. In this method, the whole computational domain is discretized using a structured (cartesian) grid. However, in spite of its flexibility and second-order accuracy in a homogeneous medium, the Yee scheme suffers from serious accuracy degradation when used to model curved objects or when treating material interfaces. During the last twenty years, numerical methods formulated on unstructured meshes have drawn a lot of attention in computational electromagnetics with the aim of dealing with irregularly shaped structures and heterogeneous media. In particular, the Discontinuous-Galerkin Time-Domain (DGTD) method has met an increased interest because these methods somehow can be seen as a crossover between Finite Element Time-Domain (FETD) methods (their accuracy depends of the order of a chosen local polynomial basis upon which the solution is represented) and Finite Volume Time-Domain (FVTD) methods (the neighboring cells are connected by numerical fluxes). Thus, DGTD methods offer a wide range of flexibility in terms of geometry (since the use of unstructured and non-conforming meshes is naturally permitted) as well as local approximation order refinement strategies, which are of useful practical interest.

In this paper, we report on our recent efforts aiming at the development of a family of high order DG-based solvers for the numerical treatment of a wide class of problems involving the interaction of light with matter at the nanoscale. Although we concentrate here on a presentation of the basic ingredients and characteristics of a DG method for time-domain nanophotonics/plasmonics applications in the linear regime assuming local dispersion effects for metallic nanostructures, we note that the present work falls within a global approach which aims at considering more general physical settings as outlined in the conclusion of the paper. The basic ingredient of a DG-based solver is a discretization method which relies on a compact stencil high order interpolation of the electromagnetic field components within each cell of an unstructured tetrahedral mesh. This piecewise polynomial numerical approximation is allowed to be discontinuous from one mesh cell to another, and the consistency of the global approximation is obtained thanks to the definition of appropriate numerical traces of the fields on a face shared by two neighboring cells. Time integration is achieved using an explicit scheme and no global mass matrix inversion is required to advance the solution at each time step. Moreover, the resulting time-domain solver is particularly well adapted

to parallel computing. The proposed method is an extension of the so-called DGTD (Discontinuous Galerkin Time-Domain) method that we initially proposed in [1] for the simulation of electromagnetic wave propagation in non-dispersive heterogeneous media at microwave frequencies. Various methodological aspects and variants of the method have been further developed in view of enhancing its accuracy and efficiency [5–9]. For the numerical treatment of dispersion models in metals, we have adopted an Auxiliary Differential Equation (ADE) technique that has already proven its effectiveness in the FDTD framework. From the mathematical point of view, this amounts to solve the time-domain Maxwell equations coupled to a system of *ordinary differential equations*. The resulting ADE-based DGTD method is detailed in [10].

2. GENERALITIES ABOUT THE DGTD METHOD

The DGTD method can be considered as a finite element method where the continuity constraint at an element interface is released. While it keeps almost all the advantages of the finite element method (large spectrum of applications, complex geometries, etc.), the DGTD method has other nice properties which explain the renewed interest it gains in various domains in scientific computing:

- It is naturally adapted to a high order approximation of the unknown field. Moreover, one may increase the degree of the approximation in the whole mesh as easily as for spectral methods but, with a DGTD method, this can also be done locally, i.e., at the mesh cell level. In most cases, the approximation relies on a polynomial interpolation method but the method also offers the flexibility of applying local approximation strategies that best fit to the intrinsic features of the modeled physical phenomena.
- When the discretization in space is coupled to an explicit time integration method, the DG method leads to a block diagonal mass matrix independently of the form of the local approximation (e.g., the type of polynomial interpolation). This is a striking difference with classical, continuous FETD formulations. Moreover, the mass matrix is diagonal if an orthogonal basis is chosen.
- It easily handles complex meshes. The grid may be a classical conforming finite element mesh, a non-conforming one or even a hybrid mesh made of various elements (tetrahedra, prisms, hexahedra, etc.). The DGTD method has been proven to work well with highly locally refined meshes. This property makes the DGTD method more suitable to the design of a *hp*-adaptive solution strategy (i.e., where the characteristic mesh size h and the interpolation degree p changes locally wherever it is needed).
- It is flexible with regards to the choice of the time stepping scheme. One may combine the discontinuous Galerkin spatial discretization with any global or local explicit time integration scheme, or even implicit, provided the resulting scheme is stable.
- It is naturally adapted to parallel computing. As long as an explicit time integration scheme is used, the DGTD method is easily parallelized. Moreover, the compact nature of method is in favor of high computation to communication ratio especially when the interpolation order is increased.

As in a classical finite element framework, a discontinuous Galerkin formulation relies on a weak form of the continuous problem at hand. However, due to the discontinuity of the global approximation, this variational formulation has to be defined at the element level. Then, a degree of freedom in the design of a discontinuous Galerkin scheme stems from the approximation of the boundary integral term resulting from the application of an integration by parts to the element-wise variational form. In the spirit of finite volume methods, the approximation of this boundary integral term calls for a numerical flux function which can be based on either a centered scheme or an upwind scheme, or a blend of these two schemes.

In the early 2000's, DGTD methods for time-domain electromagnetics have been first proposed by mainly three groups of researchers. One of the most significant contributions is due to Hesthaven and Warburton [11] in the form of a high order nodal DGTD method formulated on unstructured simplicial meshes. The proposed formulation is based on an upwind numerical flux, nodal basis expansions on a triangle (2D case) and a tetrahedron (3D case) and a Runge-Kutta time stepping scheme. In [12], Kakbian et al. describe a rather similar approach. More precisely, the authors develop a parallel, unstructured, high order DGTD method based on simple monomial polynomials for spatial discretization, an upwind numerical flux and a fourth-order Runge-Kutta scheme for time

marching. The method has been implemented with hexahedral and tetrahedral meshes. Finally, a high order nodal DGTD method formulated on unstructured simplicial meshes has also been proposed in the same time frame by Fezoui et al. [1]. However, contrary to the DGTD methods discussed in [11] and [12], the method proposed in [1] is non-dissipative thanks to a combination of a centered numerical flux with a second-order leap-frog time stepping scheme.

3. DGTD METHOD FOR TIME-DOMAIN NANOPHOTONICS

3.1. Overview of Related Works

Numerical modeling of electromagnetic wave propagation in interaction with metallic nanostructures at optical frequencies requires to solve the system of Maxwell equations coupled to appropriate models of physical dispersion in the metal. In general, the Drude and Drude-Lorentz models are adopted although there are practical situations for which these models can fail to describe correctly the behavior of some materials (e.g., transition metals [13, 14] and graphene [15]). Furthermore at some scales, non-local effects starts to play an important role [16]. As mentioned previously, the FDTD [4] method is a widely used approach for solving the systems of partial differential equations modeling nanophotonic applications. In this method, the whole computational domain is discretized using a structured (cartesian) grid. In spite of its flexibility and second-order accuracy in a homogeneous medium, the Yee scheme suffers from serious accuracy degradation when used to model curved objects or when treating material interfaces. Indeed, the so-called stair-casing approximation may lead to local zeroth-order and at most first-order accuracy; it may also produce locally non-convergent results [17]. Furthermore, for Maxwell's equations with discontinuous coefficients, the Yee scheme might not be able to capture the possible discontinuity of the solution across the interfaces [17].

Thus, with all their features (as described above), DGTD methods seem to be well suited to the numerical simulation of complex time-domain electromagnetic wave propagation problems. As a matter of fact, the DGTD method for solving the time domain Maxwell equations is increasingly adopted by several physics communities. Concerning nanophotonics, unstructured mesh based DGTD methods have been developed and have demonstrated their potentialities for being considered as viable alternatives to the FDTD method [18–23]. The most remarkable achievements in the recent years are probably those of researchers in the nanophotonics domain. The group of Kurt Busch [24–27] at the Institut für Theoretische Festkörperphysik of the Karlsruhe Institute of Technology (KIT) has been at the origin of seminal works on the development and application of the DGTD method in this domain. Noteworthy, all these studies adopt a diffusive DGTD formulation based on upwind numerical fluxes. Besides, several studies have already been conducted regarding the development of DGTD methods for dispersive media, such as [20–28]. Furthermore one can find more studies focused on numerical analysis aspects concerning dispersive media [29, 30].

3.2. A Non-dissipative DGTD Method

Towards the general aim of being able to consider concrete physical situations relevant to nanophotonics, one has to take into account in the numerical treatment, a better description of the propagation of waves in realistic media. The physical phenomenon that one has to consider in the first instance here is dispersion. In the presence of an electric field the medium cannot react instantaneously and thus presents an electric polarization of the molecules or electrons that itself influences the electric displacement. In the case of a linear homogeneous isotropic media, there is a linear relation between the applied electric field and the polarization. However, above some range of frequencies (depending on the considered material), the dispersion phenomenon cannot be neglected and the relation between the polarization and the applied electric field becomes complex. In practice, this is modeled by a frequency dependent complex permittivity. Several such models for the characterization of the permittivity exist; they are established by considering the equation of motion of the electrons in the medium and making some simplifications.

There are mainly two ways of handling the frequency dependent permittivity in the framework of time-domain simulations, both starting from models defined in the frequency domain. A first approach is to introduce the polarization vector as an unknown field through an auxiliary differential equation which is derived from the original model in the frequency domain by means of an inverse Fourier transform. This is called the *Direct Method* or *Auxiliary Differential Equation* (ADE) formulation. Let us note that while the new equations can be easily added to any time-domain Maxwell solver, the resulting set of differential equations is tied to the particular choice of dispersive model and will never act as a black box able to deal with other models. In the second approach, the

electric field displacement is computed from the electric field through a time convolution integral and a given expression of the permittivity which formulation can be changed independently of the rest of the solver. This is called the *Recursive Convolution Method* (RCM).

Given the above-mentioned approaches, the non-dissipative DGTD method initially introduced in [1] has been adapted to deal with various dispersion models. An ADE formulation has been adopted. The resulting ADE-based DGTD method is detailed in [10] where we also study the stability and a priori convergence of the method. We first considered the case of Drude and Drude-Lorentz models and, further extend the proposed ADE-based DGTD method to be able to deal with a generalized dispersion model in which we make use of a Padé approximant to fit an experimental permittivity function. The numerical treatment of such a generalized dispersion model is also presented in [10]. We outline below the main characteristics of the proposed DGTD approach in the case of the Drude model. The latter is associated to a particularly simple theory that successfully accounts for the optical and thermal properties of some metals. In this model, the metal is considered as a static lattice of positive ions immersed in a free electrons gas. Those electrons are considered to be the valence electrons of each metallic atom, that got delocalized when put into contact with the potential produced by the rest of the lattice atoms. In the case of the Drude model, the frequency dependent permittivity is given by $\varepsilon_r(\omega) = \varepsilon_\infty - \frac{\omega_d^2}{\omega^2 + i\omega\gamma}$ where ε_∞ represents the core electrons contribution to the relative permittivity ε_r , γ is a coefficient linked to the electron/ion collisions representing the friction experienced by the electrons and $\omega_d = \sqrt{\frac{n_e e^2}{m_e \varepsilon_0}}$ (m_e is the electron mass, e the electronic charge and n_e the electronic density) is the plasma frequency of the electrons. Considering a constant permeability and a homogeneous and isotropic medium, one can write the Maxwell equations as

$$\text{rot}(\mathbf{H}) = \frac{\partial \mathbf{D}}{\partial t}, \quad \text{rot}(\mathbf{E}) = -\frac{\partial \mathbf{B}}{\partial t}, \quad (1)$$

along with the constitutive relations $\mathbf{D} = \varepsilon_0 \varepsilon_\infty \mathbf{E} + \mathbf{P}$ and $\mathbf{B} = \mu_0 \mathbf{H}$, which can be combined to yield

$$\text{rot}(\mathbf{E}) = -\mu_0 \frac{\partial \mathbf{H}}{\partial t}, \quad \text{rot}(\mathbf{H}) = \varepsilon_0 \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} + \frac{\partial \mathbf{P}}{\partial t}. \quad (2)$$

In the frequential domain the polarization $\mathbf{P}$ is linked to the electric field through the relation $\hat{\mathbf{P}} = -\frac{\varepsilon_0 \omega_d^2}{\omega^2 + i\gamma_d \omega} \hat{\mathbf{E}}$, where $\hat{\cdot}$ denotes the Fourier transform of the time-domain field. An inverse Fourier transform gives

$$\frac{\partial^2 \mathbf{P}}{\partial t^2} + \gamma_d \frac{\partial \mathbf{P}}{\partial t} = \varepsilon_0 \omega_d^2 \mathbf{E}. \quad (3)$$

By defining the dipolar current vector $\mathbf{J}_p = \frac{\partial \mathbf{P}}{\partial t}$, (2)–(3) can be rewritten as

$$\begin{aligned} \mu_0 \frac{\partial \mathbf{H}}{\partial t} &= -\nabla \times \mathbf{E}, \quad \varepsilon_0 \varepsilon_\infty \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J}_p, \\ \frac{\partial \mathbf{J}_p}{\partial t} + \gamma_d \mathbf{J}_p &= \varepsilon_0 \omega_d^2 \mathbf{E}. \end{aligned} \quad (4)$$

Recalling the definitions of the impedance and light velocity in vacuum, $Z_0 = \sqrt{\mu_0/\varepsilon_0}$ and $c_0 = 1/\sqrt{\varepsilon_0 \mu_0}$, and introducing the following substitutions, $\tilde{\mathbf{H}} = Z_0 \mathbf{H}$, $\tilde{\mathbf{E}} = \mathbf{E}$, $\tilde{\mathbf{J}}_p = Z_0 \mathbf{J}_p$, $\tilde{t} = c_0 t$, $\tilde{\gamma}_d = \gamma_d/c_0$ and $\tilde{\omega}_d^2 = \omega_d^2/c_0^2$, it can be shown that system (4) can be normalized to yield

$$\begin{aligned} \frac{\partial \tilde{\mathbf{H}}}{\partial \tilde{t}} &= -\nabla \times \tilde{\mathbf{E}}, \quad \varepsilon_\infty \frac{\partial \tilde{\mathbf{E}}}{\partial \tilde{t}} = \nabla \times \tilde{\mathbf{H}} - \tilde{\mathbf{J}}_p, \\ \frac{\partial \tilde{\mathbf{J}}_p}{\partial \tilde{t}} + \tilde{\gamma}_d \tilde{\mathbf{J}}_p &= \tilde{\omega}_d^2 \tilde{\mathbf{E}}, \end{aligned} \quad (5)$$

knowing that $\mu_0 c_0/Z_0 = 1$ and $\varepsilon_0 c_0 Z_0 = 1$. From now on, we omit the $\tilde{X}$ notation for the normalized variables. The extension of the DGTD- $\mathbb{P}_p$ method formulated for non-dispersive media to the Maxwell-Drude Equation (5) is straightforward. Indeed, the last equation of (5) can be discretized as

$$\frac{1}{\Delta t} \left(\bar{\mathbf{J}}_i^{n+\frac{3}{2}} - \bar{\mathbf{J}}_i^{n+\frac{1}{2}} \right) = -\gamma_d \bar{\mathbf{J}}_i^{n+\frac{1}{2}} + \omega_d^2 \bar{\mathbf{E}}_i^{n+1}.$$

The discrete equations for a cell c_i can then be written as

$$\begin{cases} \mathbb{M}_i \left(\frac{\bar{\mathbf{H}}_i^{n+\frac{3}{2}} - \bar{\mathbf{H}}_i^{n+\frac{1}{2}}}{\Delta t} \right) = -\mathbb{K}_i \bar{\mathbf{E}}_i^{n+1} + \sum_{k \in \mathcal{V}_i} \mathbb{S}_{ik} \bar{\mathbf{E}}_k^{n+1}, \\ \mathbb{M}_i^{\varepsilon_\infty} \left(\frac{\bar{\mathbf{E}}_i^{n+1} - \bar{\mathbf{E}}_i^n}{\Delta t} \right) = \mathbb{K}_i \bar{\mathbf{H}}_i^{n+\frac{1}{2}} - \sum_{k \in \mathcal{V}_i} \mathbb{S}_{ik} \bar{\mathbf{H}}_k^{n+\frac{1}{2}} - \mathbb{M}_i \bar{\mathbf{J}}_i^{n+\frac{1}{2}}, \\ \frac{\bar{\mathbf{J}}_i^{n+\frac{3}{2}} - \bar{\mathbf{J}}_i^{n+\frac{1}{2}}}{\Delta t} = \omega_d^2 \bar{\mathbf{E}}_i^{n+1} - \frac{\gamma_d}{2} \left(\bar{\mathbf{J}}_i^{n+\frac{3}{2}} + \bar{\mathbf{J}}_i^{n+\frac{1}{2}} \right). \end{cases}$$

The stability and a priori convergence properties of the resulting ADE-based DGTD- $\mathbb{P}_p$ solver are analyzed in [10].

4. NUMERICAL AND PERFORMANCE RESULTS

In view of simulating large-scale three-dimensional problems, the computer implementation of the method has been adapted to distributed memory parallel computing platforms by adopting a widely adopted SPMD (Single Program Multiple Data) coarse grain parallelization strategy combining a partitioning of the mesh into K submeshes using the MeTiS [31] library and a message passing programming with the MPI standard. In this strategy, each of the K submeshes is treated by a single computing unit (core). Each core applies the numerical kernels of the DGTD method on the data associated to each submesh K and communication operations occur are performed for exchanging problem unknowns attached to elements on artificial interfaces between neighboring submeshes (i.e., submeshes K and K' sharing faces of these tetrahedra).

We illustrate the possibilities of the proposed DGTD- $\mathbb{P}_p$ solver by considering a setting relevant to optical communications. The selected problem involves an L-shaped waveguide inspired by [32,33]. This L-shaped waveguide is formed of seven 50 nm diameter gold nanospheres in vacuum, with a 75 nm center-to-center spacing while the whole computational domain consists of a 550 nm $\times$ 750 nm $\times$ 400 nm parallelepipedic domain. A Silver-Müller absorbing boundary condition is applied on the surface of this parallelepipedic domain. When excited by an optical regime source, the interest of this setting is the subwavelength energy guiding, from sphere to sphere, due to the surface plasmons coupling with each other. It follows that the geometry of the spheres should be correctly approximated in order to avoid non-physical energy concentration phenomena in spurious wedges of the mesh. Moreover, the vicinity of the spheres should be accurately resolved in order to capture the subwavelength phenomena of interest. Finally, the physical time window of the computation should be long enough for the phenomenon to settle. This test problem has been simulated using a DGTD- $\mathbb{P}_2$ method applied on a fully tetrahedral mesh. The constructed mesh is partially visualized on Figure 1. It consists of 222,175 vertices and 1,306,356 tetrahedra. The source term is a dipole localized in the tetrahedral subdomain, 75 nm away from the center of the first sphere in the guide. This dipolar source amounts to imposing a current density of the form $J_x((x, y, z, t) = \delta(x - x_s, y - y_s, z - z_s)f(t)$ with $f(t) = (1 - e^{-(t/\alpha)^2}) \sin(2\pi f_c t)$ where the central frequency is $f_c = 622.65$ THz, $\gamma = 2.5 \times 10^{16}$, and $\alpha = 2.5833$ fs. The parameters of the Drude model for the gold nanospheres are $\varepsilon_\infty = 1$, $\omega_d = 6.79 \times 10^3$ THz and $\gamma_d = 2.5 \times 10^2$ THz. Timesteps

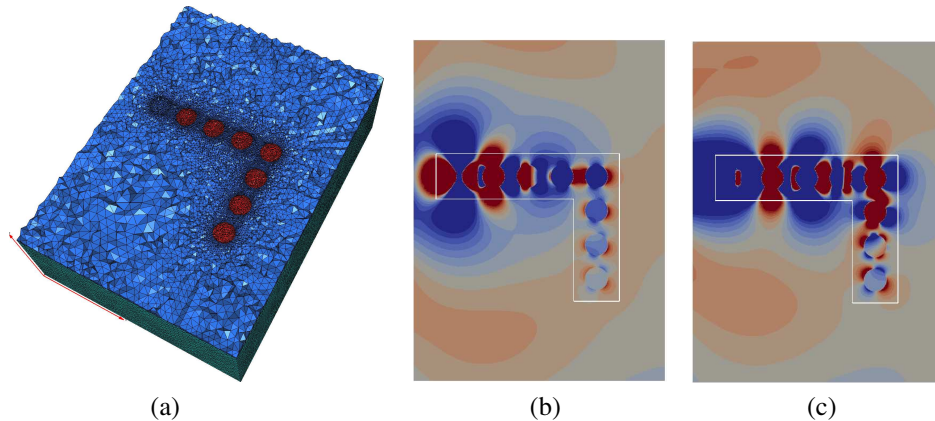


Figure 1: Simulation of an L-shaped waveguide. Partial view of the tetrahedral mesh used for the simulation of (a) the L-shaped waveguide, E_x component of the electric field for DGTD- $\mathbb{P}_2$ solution (b) at time $t = 6.02$ fs and (c) at final time $t_f = 34.13$ fs.

for these simulations are $\Delta t_h = 3.9 \times 10^{-4}$ fs and $\Delta t_t = 3.7 \times 10^{-4}$ fs.

Simulations have been performed in parallel execution mode on a cluster of Intel Xeon 2.66 GHz nodes (each consisting of 8 computing cores and 32 Gb of RAM), interconnected by an Infiniband network. Performance results are given in Table 1 for up to 128 cores. The parallel speedups are satisfying in spite of the difficulty of achieving an optimal load balancing for such an unstructured tetrahedral mesh. Finally, Figure 1 shows physical results in the form of contour lines of the E_z component on the $z = 0$ plane, first, after 6.02 fs as the resonances start to settle, and second, after 34.13 fs as the phenomenon is well-established.

Table 1: Simulation of an L-shaped waveguide. Performance results of the DGTD- $\mathbb{P}_2$ method: CPU time to reach 1 fs and parallel speedup (in parentheses).

8 cores	16 cores	32 cores	64 cores	128 cores
11420 s	5710 s	2800 s	1455 s	762 s
(1.0)	(2.0)	(4.1)	(7.8)	(15.0)

5. CONCLUSION

The work described here is part of a larger initiative aiming at the development of a software suite dedicated to nanophotonics/nanoplasmonics that will ideally include DG-based solvers for both time-domain and frequency-domain problems, as well as the capabilities to numerically consider various material models in the linear and non-linear regimes, considering local and non-local dispersion effects.

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