High order discontinuous Galerkin methods for time-domain and frequency-domain nanophotonics

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Abstract. The discontinuous Galerkin (DG) method is a general numerical modeling approach that has been extensively studied in the last 20 years for the solution of many systems of partial differential equations in physics. Its development for the numerical treatment of the system of Maxwell equations was initiated by the applied mathematics community in the early 2000s. It is now a very popular method for time-domain electromagnetics, which is increasingly used and further developed by the applied physics and electrical engineering communities. More recently, a specific variant of DG, referred to as hybridized DG (or HDG), has been proposed for frequency-domain electromagnetics. DG methods possess nice features that make them particularly attractive for dealing with heterogeneous media and irregularly shaped or curved geometries, and more generally with multiscale problems. Not surprisingly, the method has also been adopted by researchers in the nano-optics field. In this paper, we report on our recent efforts for extending the capabilities of this family of methods for the numerical modeling of nanoscale light-matter interactions.

1. Generalities about the DG method

A DG method can be considered as a finite element (FE) method in which the continuity constraint at an element interface is released. While it keeps almost all the advantages of a FE method (large spectrum of applications, complex geometries, etc.), a DG method has other nice properties, which explain its increasing popularity in the computational electromagnetics field:

- It leverages 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 DG method, this can also be done locally i.e. at the mesh cell level. In most cases, the approximation relies on a polynomial interpolation, however the method also offers the flexibility of applying local approximation strategies that best fit to the intrinsic features of the modeled physical phenomena, e.g., by using a plane wave basis expansion.

- In a time-domain setting, 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 FE formulations. Moreover, the mass matrix is diagonal if an orthogonal basis is chosen.

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- 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.). DG methods have been proven to work well with highly locally refined meshes. This property makes a DG 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).

As in a classical FE framework, a DG 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 DG 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, which have been extensively developed by hyperbolic systems of conservation laws, 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, DG methods have been studied in the context of time-domain electromagnetics. The resulting formulation is known as the DGTD (Discontinuous Galerkin Time-Domain). Such DGTD methods are described in [1] (for a formulation based on an upwind numerical flux and a Runge-Kutta time stepping scheme) and [2] (for a formulation based on a centered numerical flux and a Leap-Frog time stepping scheme). In the nanophotonics field, the DGTD method has been popularized by K. Busch et al. [3].

2. DGTD methods for time-domain nanophotonics

Towards the general aim of being able to consider concrete physical situations relevant to nanophotonics, one of the most important features to take into account in the numerical treatment is physical dispersion. In practice, this is modeled by a frequency-dependent complex permittivity. Several such models for the characterization of the permittivity exist, such as the Drude and Drude-Lorentz models for plasmonics [4], which 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 (ADE) which is derived from the original model in the frequency-domain by means of an inverse Fourier transform. 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).

In [5], we propose and analyze a high order ADE-DGTD method for solving teh system of 3D time-domain Maxwell equations coupled to a Generalized Dispersion Model (GDM) for nanophotonics and nanoplasmonics simulations. Given an experimental set of points describing a permittivity function of a material, a Padé type approximation is a convenient analytical coefficient-based function to approach experimental data. The fundamental theorem of algebra allows to expand this approximation as a sum 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), as

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

where $\varepsilon_\infty$, $\sigma$, $(a_l)_{l\in L_1}$, $(b_l)_{l\in L_1}$, $(c_l)_{l\in L_2}$, $(d_l)_{l\in L_2}$, $(e_l)_{l\in L_2}$, $(f_l)_{l\in L_2}$ are real constants, and $L_1$, $L_2$ are non-overlapping sets of indices. The constant $\varepsilon_\infty$ represents the permittivity at infinite frequency, and $\sigma$ the conductivity. This general writing allows an important flexibility for
generalized dispersive model in time-domain inverse Fourier transform, one derives the system of differential equations accounting for the dynamics of the components of $\hat{\mathbf{E}}$, $\hat{\mathbf{H}}$, and $\hat{\mathbf{P}}$.

In order to fit the coefficients of (1) to experimental data, various techniques can be used, such as the well-known least square method. In practice, for a given model, a set of experimental data is provided to the optimization algorithm [6].

In the frequency-domain the polarization $\hat{\mathbf{P}}$ is linked to the electric field through the relation $\hat{\mathbf{P}} = \varepsilon_{r,g}(\omega)\hat{\mathbf{E}}$ where $\hat{\cdot}$ denotes the Fourier transform of the time-domain field. By applying an inverse Fourier transform, one derives the system of differential equations accounting for the generalized dispersive model in time-domain

$$
\begin{align*}
\frac{\partial \hat{\mathbf{H}}}{\partial t} &= -\nabla \times \hat{\mathbf{E}}, & \frac{\partial \hat{\mathbf{E}}}{\partial t} &= \frac{1}{\varepsilon_\infty} \left( \nabla \times \hat{\mathbf{H}} - \mathbf{J}_0 - \sum_{l \in L_1} \mathbf{J}_l - \sum_{l \in L_2} \mathbf{J}_l \right), \\
\mathbf{J}_0 &= (\sigma + \sum_{l \in L_2} d_l) \mathbf{E}, & \mathbf{J}_j &= a_l \mathbf{E} - b_l \mathbf{P}_l \quad \forall l \in L_1, \\
\frac{\partial \mathbf{P}_l}{\partial t} &= \mathbf{J}_l \quad \forall l \in L_1, & \frac{\partial \mathbf{J}_l}{\partial t} &= (c_l - d_l f_l) \mathbf{E} - f_l \mathbf{J}_l - e_l \mathbf{P}_l \quad \forall l \in L_2, \\
\frac{\partial \mathbf{P}_l}{\partial t} &= d_l \mathbf{E} + \mathbf{J}_l \quad \forall l \in L_2.
\end{align*}
$$

In the above system, $\mathbf{E}_i$ is the vector of all the degrees of freedom of $\mathbf{E}$ in $\tau_i$ (with similar definitions for $\hat{\mathbf{H}}_l$ and $\hat{\mathbf{J}}_l$), $\mathbf{M}_i$ and $\mathbf{M}_i^\infty$ are local mass matrices, $\mathbf{K}_i$ is a local pseudo-stiffness matrix, and $\mathbf{S}_{ik}$ is a local interface matrix. Moreover, $\mathbf{E}_a$ and $\mathbf{H}_a$ are numerical traces computed using an appropriate centered or upwind scheme. The main features of the DGTD method that we consider are the following: It is formulated on an unstructured tetrahedral mesh; It can deal with linear or curvilinear elements through a classical isoparametric mapping adapted to the DG framework (see [7] for more details); It relies on a high order nodal (Lagrange) interpolation of the components of $\mathbf{E}$, $\mathbf{H}$ and $\mathbf{J}_p$ within a tetrahedron, which can be defined at the local cell level[8]; It offers the possibility of using a fully centered [2] or a fully upwind [1] scheme, as well as blend of the two schemes, for the evaluation of the numerical traces (also referred as numerical fluxes) of the $\mathbf{E}$ and $\mathbf{H}$ fields at inter-element boundaries; It can be coupled to several variants of a fourth-order low-storage Runge-Kutta (LSRK) time integration scheme as the ones studied in [9]; It can rely on a Silver-Müller absorbing boundary condition or a CFS-PML technique for the artificial truncation of the computational domain; It is parallelized using a classical SPMD (Single Program Multiple Data) strategy combining a partitioning of the underlying tetrahedral mesh, with a message passing programming model using the MPI standard.

Moreover, when it comes to very small structures in a regime of 2 nm to 25 nm, non-local effects due to electron collisions have to be taken into account. Non-locality leads to additional, general non-linear, partial differential equations and is significantly more difficult to treat, though. A linearized hydrodynamic fluid model, also known as the hydrodynamic Drude model [10], can be adopted for the numerical treatment of such spatial dispersion effects. We have proposed DGTD methods for solving the system of Maxwell equations coupled to a linearized hydrodynamic Drude model in [11] (2D case) and [12] (3D case).

3. HDG methods for frequency-domain nanophotonics

When dealing with the simulation of the propagation of time-harmonic electromagnetic waves in heterogeneous media, the FE method [13] based on so-called edge element basis expansions [14] is
the method of choice. For the numerical treatment of the frequency-domain Maxwell equations, classical DG methods can also be considered [15]. However, such DG formulations are highly expensive, especially for the discretization of three-dimensional problems, because they lead to a large sparse and indefinite linear system of equations coupling all the degrees of freedom of the unknown physical fields. As a consequence, the number of globally coupled DG degrees of freedom is much greater than the number required by conforming finite element methods for the same accuracy. Different attempts have been made in the recent past to improve the efficiency of DG methods applied to steady-like problems and one promising strategy has been proposed by Cockburn et al. [16] in the form of so-called hybridizable discontinuous Galerkin (HDG) formulations.

HDG methods introduce an additional hybrid variable on the faces of the elements, on which the definition of the local (element-wise) solutions is based. A so-called conservativity condition is imposed on the numerical trace, whose definition involved the hybrid variable, at the interface between neighboring elements. As a result, HDG methods produce a linear system in terms of the DOFs of the additional hybrid variable only. In this way, the number of globally coupled DOFs is reduced. The local values of the electromagnetic fields can be obtained by solving local problems element-by-element. Such a HDG method has been proposed for the solution of the 3D frequency-domain (or time-harmonic) Maxwell equations in [17], which is combined to a domain decomposition (DD) based hybrid iterative-direct parallel solution strategies. We have recently adapted it to the context of nanophotonics and nanoplasmonics, in particular by taking into account a frequency-dependant permittivity (1).

4. Conclusion
The work described here is part of a larger initiative aiming at the development of a software suite dedicated to nanophotonics and nanoplasmonics that 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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