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Simulation de la propagation d'ondes électromagnétiques en nano-optique par une méthode Galerkine discontinue d'ordre élevé

Simulation of electromagnetic waves propagation in nano-optics with a high-order discontinuous Galerkin time-domain method

Thèse dirigée par Stéphane Lanteri & Claire Scheid
soutenue le 10 décembre 2015

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"La vie ce n'est pas d'attendre que les orages passent, c'est d'apprendre à danser sous la pluie"

— Sénèque

Acknowledgements

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1
Introduction

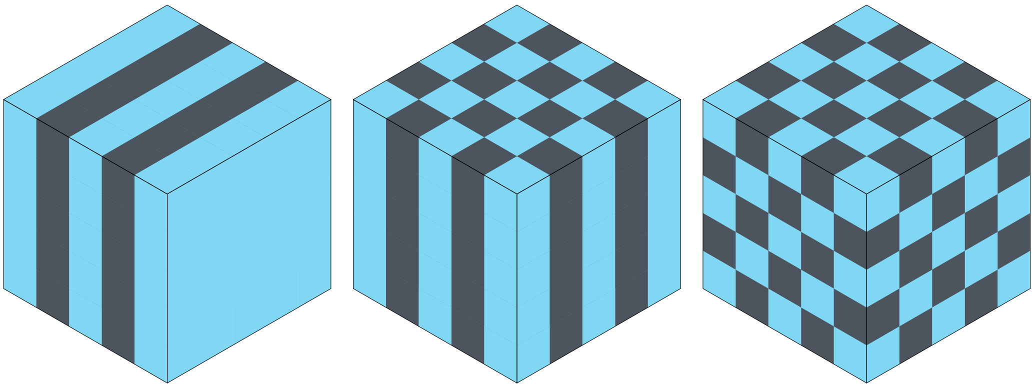
1.1 A bit of History

The first observations of electric and magnetic phenomena by man date back to 600 B.C., when Thales of Miletus observed the property of amber to attract light objects, such as fabric, after being rubbed with fur. In the same period, he also reported the existing attraction between lodestone and iron. Three centuries later, Euclid threw together the basis of geometrical optics in *Optica*, describing the laws of reflection and postulating that light travels in straight lines. From this point, the studies of electromagnetism and light followed parallel paths, until the XIX$^{\text{th}}$ century. In 1848 and 1850, Hippolyte Fizeau and Léon Foucault measured the speed of light respectively at 3.14×10^8 and 2.98×10^8 m.s^{-1}. In 1855, Wilhelm Eduard Weber and Rudolf Kohlrausch found out through an experimentation that the ratio of the electromagnetic to the electrostatic unit charge was close to 3.107×10^8 m.s^{-1}. Although the values from Fizeau and Foucault were known at that time, they did not notice the alikeness of the results [Kei98].

It is only in 1861 that James Clerk Maxwell, looking at Weber and Kohlrausch's results, established the existing link between light propagation and electromagnetic phenomena. In [Max65], he concludes : "The agreement of the results seems to show that light and magnetism are affections of the same substance, and that light is an electromagnetic disturbance propagated through the field according to electromagnetic laws". At that stage, Maxwell's theory of electromagnetism is regrouped in a set of twenty unknowns and equations, that will then be converted into modern notations by a concurrent work of Olivier Heaviside, Josiah Willard Gibbs and Heinrich Hertz in 1884. It should be noted that the 1861 formulation of Maxwell still relies on the existence of the luminiferous aether, a postulated medium necessary to the propagation of light. For more than forty years, the latter will be a source of conflict, his properties being very difficult to accept in the physical paradigm of that time. In 1905, Einstein's special theory of relativity finally provided a framework that did not require the presence of aether anymore.

1.2 Nano-optics

Maxwell's equations in their modern form have been studied for many decades, resulting in an extremely wide range of applications. Many of those are now part of our everyday life, such as wireless communications of all forms, optical fibers, medical imaging, ... In order to control electromagnetic wave propagation, most of these devices rely on tailored geometries and materials. During the last decades, the evolution of lithography techniques allowed the creation of geometrical structures at the nanometer scale, thus unveiling a variety of new phenomena arising from light-matter interactions at such levels. These effects usually occur when the device is of comparable size or (much) smaller than the wavelength of the incident field. Periodic mono- or multi-dimensional arrangements of sub-wavelength dielectric patterns, known as photonic crystals (see figure 1.1), give rise to allowed and forbidden wavelengths regions in certain directions [JJ07]. These so-called band gaps can be tuned by slight modifications of the periodicity, allowing physicists to create a full range of light-control devices from photonic crystals. Periodic arrays of dielectric resonators can also be used to achieve non-cartesian reflection of plane waves, which is a highly promising step toward on-chip wireless optical communications [ZWS+13].



(a) 1D cristal (b) 2D cristal (c) 3D cristal

Figure 1.1 | **Photonic crystal structures** in one, two and three dimensions. The blue and gray areas represent the alternance of high and low permittivity materials.

Metallic nanostructures can also demonstrate stunning effects when excited in the optical regime. The key feature of these effects is the coupling of the electromagnetic field to the electron gas of the metal, resulting in an oscillation phenomenon called plasmon. One usually differentiates the bulk plasmons, that take place in the volume, from the surface plasmons (SP), that arise at the interface between the metal and a dielectric. SPs can be propagative along a metal/dielectric interface, or non-propagative, in which case they are called localized surface plasmons (LSPs). The proper excitation of LSPs can lead to very intense resonances (meaning that the field is enhanced). Thanks to metallic tips exploiting this strong localization, optical microscopy beyond the diffraction limit [NH07] is possible. The high sensitivity of resonant metallic nanostructures also allows to create very accurate biosensors [CLS+11]. In the medical field, attempts have been made to develop cancer therapies based on the localized heating produced with resonating nano particles [SSD+14]. As for dielectrics, periodic arrays of metallic patterns can lead to new devices with non-natural behaviors at larger scales. These structures are usually gathered under the root word metamaterials, which then designates an effective medium composed of an arrangement of nanostructures, and displaying uncommon properties. Negative refractive index materials [DWSL07] or optical cloaking [CCKS07] are some of the most common examples.

1.3 Computational electromagnetics in time-domain

The large variety of phenomena displayed by nano-optic systems, their dependance upon a large number of parameters (geometry, materials, sources, ...), as well as the complexity of most fabrication processes prevent physicists from relying on experiments only. However, apart from very specific cases involving simple geometries, and for which electromagnetic fields can be expressed as closed-forms, solutions to Maxwell's equations are out of reach of hand calculations. Hence, numerical simulation seems to be the appropriate complementary tool to physical experiments, and can be exploited in various ways. Indeed, it can be used to rapidly scan a large number of configurations, in order to identify the most efficient set of parameters. This scanning can be done "blindly" by hand if a small number of parameters is involved, or by combining a direct numerical method to an iterative optimization algorithm when the dimension of the parameters space becomes large [Pav13]. Numerical tools also allow a deeper understanding of the physical phenomena observed in real devices, since they allow the experimentalist to obtain information about any quantity out of the simulation, which is not possible in most physical experiments. Additionally, various physical models can be easily assessed and their effects compared, in order to verify their applicability in given configurations. Various techniques are available to solve nano-optics problems: some are specialized algorithms, that were developed for the fast-solving of specific configurations at low computational cost (for example the Discrete Dipole Approximation (DDA) [DF94] or the Rigorous Coupled-Wave Analysis (RCWA) [MG81]). However, these can hardly or not at all handle other applications. On the other hand, more general methods exist that are well suited to solve a very large set of problems. In the remaining of this section, we focus on the major time-domain techniques.

The Finite-Difference Time-Domain (FDTD) method is certainly the most spread of all. As early as 1928, Courant, Friedrichs and Lewy published an article presenting a finite-difference scheme for the second order wave equation in 1D and 2D, as well as the well-known CFL stability condition involved for explicit time-domain schemes [RFH28]. In 1966, Yee introduced a staggered grid in space (see figure 1.2) to solve the curl formulation of Maxwell's equations [Yee66]. The method relies on a combination of Taylor expansions to express the spatial derivatives, and on a centered Leap-Frog (LF) scheme in time. As of today, FD represent a particularly simple method to solve electromagnetics problems, combining simple implementation and high computational efficiency. They were applied successfully to numerous nano-optics configurations [SCG10].

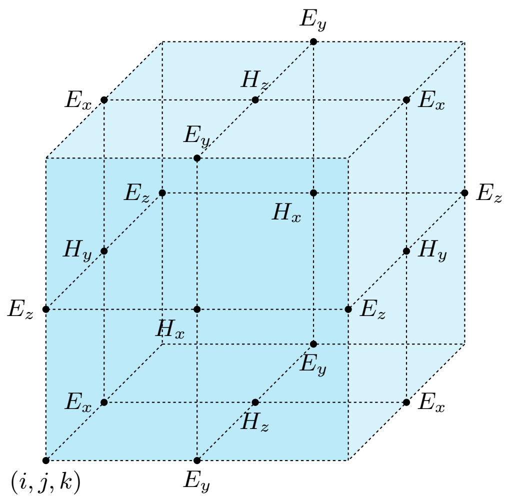


Figure 1.2 | Staggered unknowns discretization in a Yee cell. The **H** field components are on the center of the faces, while the **E** ones are on the center of the edges.

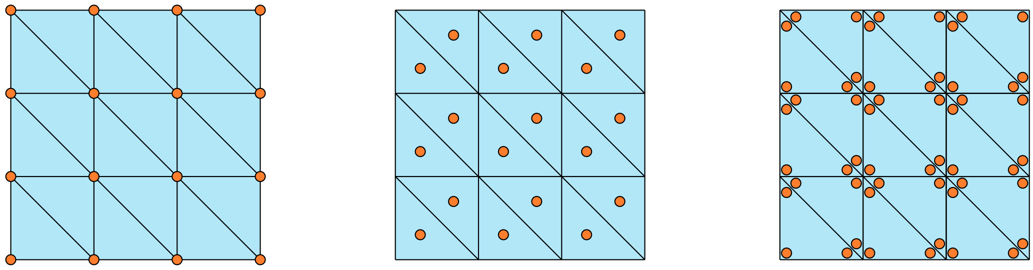
However, FD algorithms suffer from serious drawbacks. First, a smooth discretization of curved geometries is impossible due to the fixed cartesian grid imposed by the Yee algorithm. This approximation leads to the well-known staircasing effect, which is an important source of inaccuracy [DDH01]. To overcome this pitfall, the user can either use an extreme refinement of the grid, which leads to a serious rise in computational cost, or exploit one of the numerous possible modifications of the FD method that have been proposed for tackling the staircasing effect [HR98]. However, all the latter available modifications represent a tradeoff between the simplicity of the classical algorithm and the accuracy of the boundary description. The second main source of inaccuracy in the FDTD method arises in the case of heterogeneous problems. In this case, the Taylor approximation used is no longer valid, since the electromagnetic fields are not smooth across the interface. The consequence is that higher-order FD schemes in space are usually reduced to second-order. Advanced FDTD methods were developed to tackle this problem [TH05], at the price of an increased complexity of the algorithm. Moreover, there is no theoretical convergence proof for FDTD algorithms outside the uniform grid case.

Finite Elements (FE) were introduced in 1969 by Silvester to solve waveguide problems [Sil69]. This method does not rely on a grid, but on a tessellation of the geometry of the problem. Starting from the continuous equations, a discrete variational form is obtained by approximating the unknowns in a finite dimensional space. Then, its discretization leads to a sparse matrix-vector system that has to be solved at each timestep. In the specific case of electromagnetism, the use of nodal basis functions, *e.g.* such as their value is unity at a given vertex and zero on every other, is subject to caution. Indeed, it was proved that they can lead to spurious oscillations, due to an ill representation of the curl kernel [SMYC95]. To overcome this issue, Nédélec introduced a new family of vector finite elements in 1986 [N80], named Nédélec finite elements, or edge finite elements. These elements display several interesting properties: (i) their divergence is zero, and (ii) each basis function associated to an edge has a constant tangential component on the latter, and a zero tangential component on the others. Hence, the tangential continuity of the electric field across the edge is naturally enforced.

In order to adjust the accuracy of the simulation, FE methods can use either (i) a local refinement or coarsening of the mesh, (ii) a local or global increase of the order of the basis functions, or (iii) a combination of both. However, these improvements lead to larger linear systems to solve at each timestep, which can make the FE method impractical in time-domain simulations for very large systems. For this reason, in nano-optics, FE methods are more often used in frequency-domain. However, a few references can be found exploiting time-domain FE for nanophotonics applications [HLY13].

1.4 The Discontinuous Galerkin Time-Domain method

Discontinuous Galerkin (DG) methods were originally introduced in 1973 by Reed and Hill [RH73], and have been widely used since in the computational fluid dynamics field. However, their application to the time-domain Maxwell equations is more recent [RF98]. DG methods can be seen as classical finite element methods for which the global continuity of the approximation is lifted. In the same fashion as FE methods, the unknowns are approximated on a finite set of basis functions. However, for DG, the support of basis functions are restrained to a single discretization cell. Hence, the solution produced by a DG method is discontinuous (similarly to finite volumes), and multiple different field values are stored for each element/element interface degree of freedom (see figure 1.3). The three main consequences are that (i) DG methods naturally handle material and field discontinuities, (ii) the weak formulation is local to an element, implying no large mass matrix inversion in the solving process, and (iii) the order of polynomial approximation in space can be made arbitrarily high by adding more degrees of freedom inside the elements. However, this also means that DG methods have higher memory requirements than standard FE methods. Afterward, connexion between the cells is restored by the use of a numerical flux, in the fashion of finite volume methods. The choice of the numerical flux has a great influence on the mathematical properties of the DG discretization, as energy preservation, for example.



(a) Finite elements : continuous, non-constant-per-cell solution

(b) Finite volumes : discontinuous, constant-per-cell solution

(c) Discontinuous Galerkin : discontinuous, non-constant-per-cell solution

Figure 1.3 | Concept comparison between FE, FV and DG. The triangles represent the cells of the mesh, while the orange dots represent the degrees of freedom. For FE, the whole problem is considered at once, and the obtained numerical solution is continuous across cell interfaces. For FV, a local problem is considered in each cell, leading to a discontinuous, constant-per-cell solution. For DG, the method is analog to FV, but the solution is not restrained to a constant per cell. In this case, a first-order polynomial approximation is used for the DG discretization.

The discontinuity of the approximation makes room for numerous methodological improvements, such as efficient parallelization ([Die12], [BFLP06]) or the use of non-conforming [FL10] and hybrid meshes [LVD+14]. Recent studies in the DG framework include local timestepping [Pip05] as well as locally implicit formulations [Moy12]. Also, a wide choice of time-integration schemes can be used for the discretization of time derivatives, including Leap-Frog (LF) and Runge-Kutta (RK).

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. The most remarkable achievements in the nanophotonics domain since 2009 are due to Busch et al. Busch [NKSB09]-[SKNB09]-[BKN11] has been at the origin of seminal works on the development and application of the DGTD method in this domain. These works not only deal with the extension of the DGTD method with regards to the complex material models and source settings required by applications relevant to nanophotonics and plasmonics [KBN10]-[MNHB11]-[WROB13], but also to core contributions aiming at improving the accuracy and the efficiency of the proposed DGTD solvers [NKP+10]-[NDB12]-[DNBH15].

1.5 Outline

The remaining of this manuscript is structured in the following way:

- Chapter 2 presents the usual concepts of electromagnetics, as well as some standard textbook problems and their analytical solutions. An extensive presentation and analysis of dispersive models for metals follows, along with a comparison of our custom generalized dispersive model with other classical dispersion models.
- The first section of chapter 3 runs, step by step, through the spatial discretization of Maxwell's equations by the discontinuous Galerkin method. Then, two classical time integration methods are proposed and briefly studied to complete the discretization. The algorithm is then validated for classical and dispersive materials. Finally, a few theoretical results are given on the method.

- ◇ Chapter 4 regroups practical techniques that are pre-requisites for the resolution of realistic problems, such as perfectly-matched layers, sources, total-field scattered-field technique, as well as physical post-treatments.
- ◇ In chapter 5, the DG method is extended to the use of quadratic tetrahedra, which allow both a better geometrical description of the problems, and lifts the numerical accuracy limit from 2^{nd} to 4^{th} order in the case of curved geometries. Several nano-optics relevant test-cases are considered that confort the interest of this development.
- ◇ Chapter 6 is dedicated to a locally-adaptive DG formulation, where polynomial interpolation order can be defined independently in each cell of the mesh. An efficient repartition algorithm is supplied, which provides interesting speedups over homogeneous polynomial repartition in several realistic test-cases.
- ◇ The sequential and parallel performances of our Fortran discontinuous Galerkin time-domain (DGTD) implementation are assessed in chapter 7. First, a renumbering algorithm is proposed that enhances the sequential performances by reducing adressing time. Then, the speedup and parallel balance of the MPI implementation are tested on a standard cavity case.
- ◇ The last chapter is dedicated to realistic nanophotonics computations processed with our DGTD code: (i) the electron energy loss spectrum (EELS) of an aluminium nanosphere, (ii) the gap-plasmon resonances obtained under chemically-produced nanocubes with realistic shapes, and (iii) 1D and 2D dielectric reflectarrays, with study of the lithography defects on their performances.

2

Outlook

In this chapter, we go over the content of the present manuscript, and point out the future possible works that are or could be carried to progress toward more complex physics and performant computations.

2.1 Summary

The goal of this thesis was to elaborate a 3D discontinuous Galerkin time-domain code able to handle complex nano-optics configurations. In the following paragraphs, we review the content of this thesis, and point out our efforts and associated contributions toward this objective.

First, a customized generalized dispersive model was developed. This model covers a wide range of dispersive materials, and proved to be roughly twice more accurate to fit experimental data than the widespread Drude and Drude-Lorentz models, for standard metals such as gold and silver in the THz regime. A significant improvement was obtained for nickel (a transition metal) when comparing the performance of the Drude model with a single generalized pole. Finally, a short digression was made on non-local dispersive models, with preliminary results in 2D.

Then, the discontinuous Galerkin time-domain method was thoroughly developed and validated for non-dispersive and dispersive materials, and two time-stepping techniques taken from the literature were proposed. Several numerical experiments related to fluxes were conducted to complete this overview. To conclude, several theoretical proofs were given, some being the result of associated works conducted during this thesis.

The next chapter contains all the numerical developments necessary to handle the computation of realistic cases, such as perfectly-matched layers, total field/scattered field formulation, complex sources, or physical post-treatments. Although additional numerical experiments were conducted about the performances of absorbing boundary conditions and perfectly matched layers, these techniques were all adapted from the literature.

Two methodological developments were then investigated in order to improve the efficiency and the accuracy of the DGTD algorithm. First, the possibility to handle curvilinear elements was considered. This possibility is not new to the DG community, and after a presentation of the mathematical and numerical framework, our approach was resolutely oriented toward the improvements this technique could bring to nano-optics computations. Through increasingly-complex configurations, the use of curvilinear elements proved to be a serious asset in terms of performance and accuracy. In the following chapter, the possibility to exploit variable polynomial orders through the computational domain was explored. After the necessary developments and a standard validation of the implementation, an order repartition algorithm was proposed that provided interesting speedups on meshes with heterogeneous mesh sizes (with a ratio up to 1000), while the accuracy of the results is barely altered (less than 1% of relative error). However, this implementation relies on a good preliminary knowledge of the physics involved in the considered configuration. A coupling with an *a posteriori* error estimate could lift this limitation by adapting the polynomial order on-the-fly, which could also alleviate the computational cost. The coupling of the order repartition algorithm with curvilinear elements can also constitute an interesting exploration path.

In the following chapter, the sequential and parallel performances of our code were assessed. A cell-renumbering algorithm was shown to provide interesting speedups, especially for low approximation orders. After a few numerical experiments with the Metis mesh partitioning tool, the speedup and efficiency of our parallel MPI implementation was assessed on a standard test-case. Results showed that this implementation provided an acceptable scaling up to a few hundred of cores, as long as the number of cells per core remained sufficiently high (around 10,000). Computation results from other chapters also proved that there was a serious need for a better load balance between cores when complex features (PMLs, curved elements, on-the-fly Fourier transforms, ...) were used.

The final chapter aims at demonstrating the capabilities of our current DGTD implementation on realistic cases. The first case consists in the computation of the EELS spectrum of a metallic nanosphere, and was adapted from existing literature. It constitutes a preliminary step toward more advanced works dealing with the proper treatment of electron-based electromagnetic sources. The second configuration involves the gap-plasmon resonances observed under chemically-produced nanocubes on metallic plates. First, the influence of the rounding at the cube edges was demonstrated. Then, different behaviors were identified, depending on the cube side length and the thickness of the dielectric spacer. These results will constitute the base of a wider study in collaboration with A. Moreau [MCM+12]. The last case deals with 1D and 2D dielectric reflectarrays, which goal is to reflect incident light with a tunable deflection angle. First, the impact of realistic lithography flaws on the performance of a 1D array was assessed. Then, the computation of a larger 2D reflectarray is considered. These results are the first step toward a wider study on this topic in collaboration with M. Klemm [ZLGW+14].

2.2 Future works

The topics presented in this manuscript give rise to a number of possible further developments, both from the numerical and the physical point of view. We close this manuscript with a short discussion of these topics.

2.2.1 Physics and material models

The numerical treatment of the non-local model, briefly presented in section **??**, remains to be thoroughly studied in the DG framework. Because of the very small physical scale involved, 3D computations with non-local models promise to be computationally expensive, and an efficient parallel implementation would constitute a good asset to compute the response of large-scale systems.

The discretization of non-linear materials in the DG framework also remain to be explored in details. Literature on this topic is very shallow, with only a handful of references limited to 1D formulations for Kerr effects [Bla13] [FL15].

2.2.2 Numerical improvements

As was stated in the introduction, the DG method allows a large panel of methodological improvements, each presenting advantages and drawbacks. In most cases, the goal of these enrichments is either to (i) alleviate the number of degrees of freedom (hybrid [LVD+14] and non-conforming meshes [FL10]), to (ii) handle the ill time discretization induced by very small elements (local time-stepping [DG09], implicit/-explicit formulations [Moy12], space-time DG method [PFT00]), or to (iii) obtain a combination of both (hp-adaptivity [SW12]).

New numerical methods derived from the classical DG algorithm are also appearing. In the Hybridizable Discontinuous Galerkin (HDG) method, a Lagrange multiplier representing the trace of the numerical solution on the element faces is introduced. A global problem on the mesh skeletton (*i.e.* the faces of the mesh) is obtained and solved, before the volumic solution can be recovered with local, independent computations. Originally designed for the time-harmonic Maxwell's equations [NPC11], implicit time-domain HDG formulation for Maxwell's equations have been developped [LP11]. A more general technique, the Multiscale Hybrid Mixed (MHM) method [HPV13], includes the DG algorithm as an inner solver to handle large, multiscale problems. In this method, the final solution is obtained as the sum of (i) the global solution of the problem of a coarse mesh and (ii) local, independent solutions computed on finer meshes in each cell.

2.2.3 High-performance computing

To compute larger and larger nano-optics systems, one cannot solely rely on Moore's law, and needs to call upon adequate parallel implementations. As can be guessed from the results of the present manuscript, a specific effort must be made to obtain decent scalings out of very large clusters (*i.e.* from several thousands to tens of thousands). OMP- or MPI-only parallel implementations on standard CPU clusters are not likely to achieve such performances. Hybrid parallelism (MPI/OMP [LLS+14]) or specific implementations for advanced HPC architectures (cluster/booster division [LMDL15]) represent potential candidates to efficient massively parallel DG algorithms.

Publications

Research articles

- *A DGTD method for the numerical modeling of the interaction of light with nanometer scale metallic structures taking into account non-local dispersion effects*; N. Schmitt, C. Scheid, S. Lanteri, A. Moreau and J. Viquerat, submitted
- *Analysis of a generalized dispersive model coupled to a DGTD method with application to nanophotonics*; S. Lanteri, C. Scheid and J. Viquerat, submitted
- *Simulation of near-field plasmonic interactions with a local approximation order discontinuous Galerkin time-domain method*; J. Viquerat and S. Lanteri, Photonics and Nanostructures - Fundamentals and Applications, **18**, 43 – 58 (2016)
- *A 3D curvilinear discontinuous Galerkin time-domain solver for nanoscale light-matter interactions*; J. Viquerat and C. Scheid, Journal of Computational and Applied Mathematics, **289**, 37 – 50 (2015)
- *A parallel non-conforming multi-element DGTD method for the simulation of electromagnetic wave interaction with metallic nanoparticles*; R. Léger, J. Viquerat, C. Durochat, C. Scheid and S. Lanteri, Journal of Computational and Applied Mathematics, **270**, 330 – 342 (2014)
- *Recent advances on a DGTD method for time-domain electromagnetics*; S. Descombes, C. Durochat, S. Lanteri, L. Moya, C. Scheid and J. Viquerat, Photonics and Nanostructures – Fundamentals and Applications, **11**, 291 – 302 (2013)

Oral presentations

- *Curvilinear discontinuous Galerkin time-domain method for nanophotonics*; ACOMEN, Ghent (2014)
- *Discontinuous Galerkin time-domain method for nanophotonics*; META conference, Singapore (2014)
- *Discontinuous Galerkin time-domain method for nanophotonics*; WAVES conference, Tunis (2013)
- *Simulation de la propagation d'ondes électromagnétiques en nano-optique par une méthode Galerkin discontinue d'ordre élevé*; GDR Ondes GT2, Troyes (2012)

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