Modelling and simulation for nanophotonics

5-7 Oct 2016
Inria Sophia Antipolis-Méditerranée
France

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A hybridizable discontinuous Galerkin method for the simulation of nonlocal optical response

Liang Li, Stéphane Lanteri, Martijn Wubs and N. Asger Mortensen

Abstract

We propose a hybridizable discontinuous Galerkin (HDG) method for solving the frequency-domain nonlocal hydrodynamic Drude (NHD) model, which is one of the most widely adopted nonlocal response models for the description of the light-matter interactions [1, 2]. The macroscale electromagnetic waves are modeled by Maxwell's equations, while the motion of the electron gas is formulated as a hydrodynamic flow. The proposed HDG method can easily couple the two sets of equations as well as the boundary conditions on the nano material boundary. In our simulations, the open scattered field is truncated by a perfectly matched layer. Numerical tests on a nanowire [3] show that the HDG method has optimal convergence rate. Even on a coarse mesh, we can have accurate enough extinction cross section calculations with high order HDG method if curvilinear treatment is taken into account, see Figure 1.

Key words: Maxwell's equations, Nonlocal hydrodynamic Drude model, GNOR model, hybridizable discontinuous Galerkin method

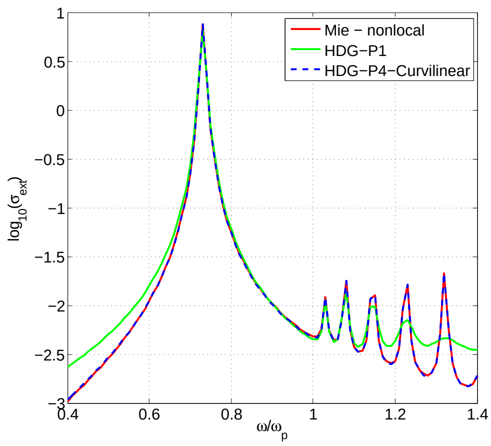

Figure 1: Extinction cross section of a sodium nanowire with radius 2 nm. The results are calculated on a mesh with 2448 triangles.

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An efficient use of polynomial subsectional basis functions in photonics and plasmonics

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August 10, 2016

In plasmonics and photonics in general, solving Maxwell equations involving irregular functions is common. For example when the relative permittivity is a piecewise constant function describing a dielectric-metal interface, the eigenmodes of the propagation equation are solutions of Maxwell's equations subject to specific boundary conditions at the interfaces between homogenous media. Prior knowledge about the eigenmodes allows to define more suitable expansion functions and the rate of convergence of the numerical scheme depends on the choice of these functions. The Fourier Modal method (FMM), consists in approximating the eigenvectors of the operator of diffraction by a partial Fourier sum. The case of metallic gratings and especially the TM polarization case challenged, for a long time, the community until calculation rules are suggested, allowing a fast convergence of the series of the partial Fourier sums. Here, we present and explain gradually, an unified numerical formalism that allows to build, from a set of subsectional functions defined on a set of subintervals, expansion functions defined on a global domain, by enforcing certain stress, deduced from electromagnetic field properties. The efficiency of the current formalism is demonstrated in a numerical modal analysis of both periodic and non-periodic plasmonic devices.

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Conformal Boundary Optics

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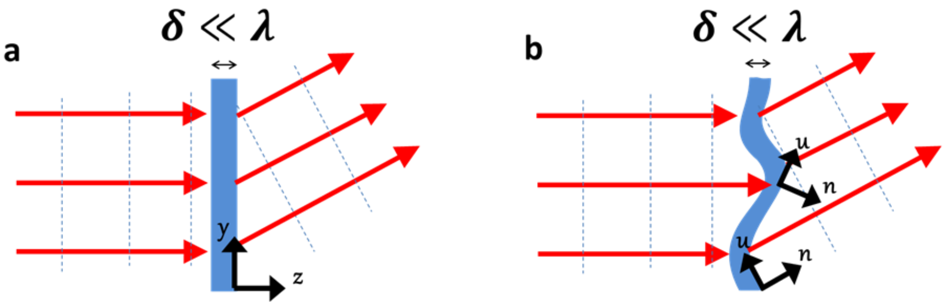
Abstract-Rapid developments in the emerging field of stretchable and conformable photonics necessitate analytical expressions for boundary conditions at metasurfaces of arbitrary geometries. We will discuss the idea of ''conformal boundary optics'': a design theory that determines the optical response for designer input and output fields at interfaces of arbitrary shapes. Given any object, one can now realise coatings to achieve exotic effects like optical illusions and anomalous diffraction behavior [1].

To date, a rigorous expression of the electromagnetic boundary conditions at designer interfaces --also called metasurfaces-- has been proposed only for planar interfaces where the electromagnetic fields are defined using a Cartesian coordinate system [2-6]. These equations are known as the generalized sheet transition conditions (GSTCs). From a physical point of view, discontinuities in electromagnetic fields across any regular surface depend upon the constitutive parameters of the interface: namely, surface charge density ρ , the current density j, the induced dipole moments at the interface and the optical response of the surrounding media. This requires (ρ, j) and the fields **E**,**H**,**p** and **m** in the Maxwell's equations to be expressed in the sense of distributions, where **E,H** are respectively the electric and magnetic fields, and **p** and **m** respectively represent the surface electric and magnetic induced currents derived by averaging the local fields of the electric and magnetic induced dipole moments in the plane z=0. In a planar configuration, writing each variable as a discontinuous function at z=0, it is possible to derive a set of generalized sheet transition conditions (GSTCs) for the electromagnetic fields [2,3]. However, this derivation is possible only because the ambient coordinate system is chosen to conform to the interface, a method that becomes very restrictive when the interface contains arbitrary contours (Fig. 1).



Figures 1: . a), a 2D planar metasurface of sub-wavelength thickness δ≪λ, can transmit any incident optical field at a specific angle by imposing a gradient of phase discontinuity. For planar interfaces, GSTC boundary conditions readily apply and the surface susceptibility tensors can be calculated. b, The local coordinate system of the surface follows its local curvature, and therefore it changes with the position

along the interface. Boundary conditions of the fields are obtained in the coordinate system of the interface, and are therefore position dependent. To produce an effect equivalent to that in b, the surface susceptibilities of the optical interface have to be engineered to account for the effect of the physical distortion. The dashed blue lines denote the equiphase fronts of the electromagnetic fields.

Here, we introduce the concept of conformal boundary optics, an analytical method – based on novel, first-principle derivations – that allows us to engineer transmission and reflection at will for any interface geometry and any given incident wave.

Whereas transformation optics determines bulk optical properties by exploiting the relationship between a given coordinate system and the coordinate system that conforms to the travel of light [7], the proposed concept determines the optical properties of a metasurface of arbitrary geometry by exploiting the relationship between a given ambient coordinate system and the coordinate system that conforms to the geometry of the boundary [1]. While a powerful concept in itself, the mathematical derivation associated with its analytical formulation is highly non-trivial since it cannot be generalized from existing boundary conditions for generic surface geometries. This concept provides a wide range of new design opportunities, for example, to hide objects behind an "optical curtain", to create optical illusions by reflecting virtual images, or to suppress the diffraction generally occurring during light scattering at corrugated interfaces.

Acknowledgements, we gratefully acknowledge financial supports from the European Research Council under grant no. 639109.

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Coupling between 3D optical and electrical simulations. Application to nanowire-based solar cells

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Abstract

In the framework of photovoltaics, increasing efforts have recently been devoted to material savings, leading to the emergence of new designs based on nanotextured [ea14a], [ea15] and nanowire-based solar cells [ea14b]. The design of devices with small absorber volumes, light-trapping nanostructures and unconventional carrier collection schemes is very demanding in term of simulation resources and cannot be performed by the opto-electronic tools already available with free or commercial licenses. In this context, we have developed new solutions for full 3D opto-electrical simulations using the most advanced optical and electrical simulation techniques. We will present an overview of its simulation capabilities and the key issues that have been solved to make it fully operational and reliable.

As an illustration of the specificity and requirement for the simulation of nanotextured solar cells, we will focus our discussion on the simulation of GaAs/AlGaAs nanowire arrays arranged in square lattice (see Figure 1a). Nanowire based solar cells are well known to efficiently absorb light with low material volumes thanks to optically resonant modes originating from individual nanowires or from the nanowire ensemble [ea14b].

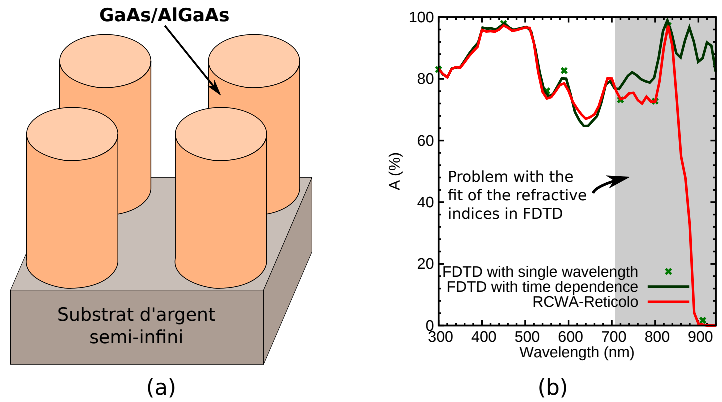

Figure 1: (a) GaAs/AlGaAs nanowire array structure, (b) issue concerning the convergence of FDTD tool due to the refractive index fitting.

In this contribution, a benchmark of optical tools using FDTD (finite difference time domain) and RCWA (rigorous coupled wave analysis) methods will firstly be performed on GaAs/AlGaAs nanowire arrays in order to determine the best candidate for the optical simulation of the nanowire array. The CPU and memory usage, advantages and limitations of both FDTD (i.e. issues concerning material refractive index fitting, as illustrated in Figure 1b) and RCWA methods (limitation concerning the geometry) will be analyzed. Then, the coupling procedure between optical and electrical software, the methodology developed to reduce the computation time and resources exploiting the cylindrical symmetry of the nanowire will be described.

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Curvilinear DGTD method for nanophotonics applications

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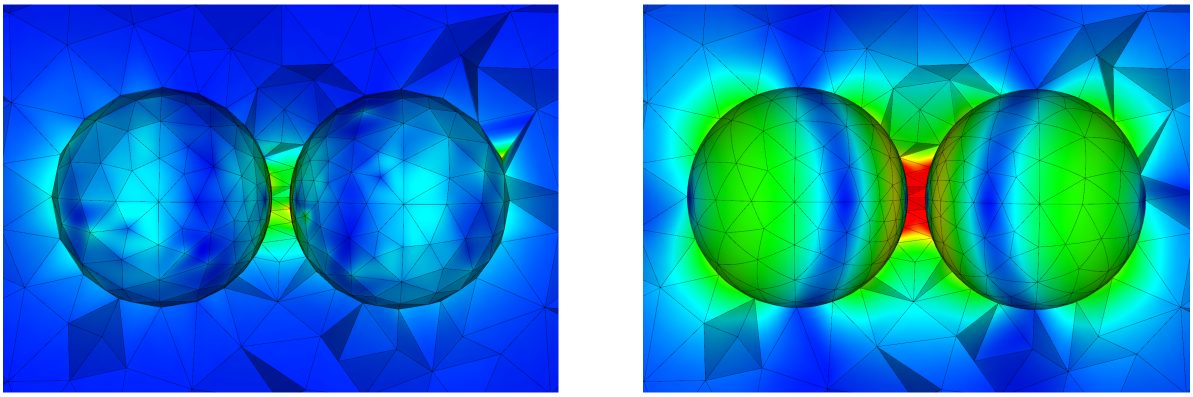
September 12, 2016

Abstract

Classical finite element methods rely on tessellations composed of straight-edged elements mapped linearly from a reference element, on domains which physical boundaries are indifferently straight or curved. This approximation represents serious hindrance for high-order methods, since they limit the precision of the spatial discretization to second order. Thus, exploiting an enhanced representation of the physical geometry of a considered problem is in agreement with the natural procedure of high-order methods, such as the discontinuous Galerkin method. In the latter framework, we propose and validate an implementation of a high-order mapping for tetrahedra, and then focus on specific nanophotonics setups to assess the gains of the method in terms of memory and performances.

The discontinuous Galerkin time-domain (DGTD) methods rely on a linear mapping from a straight reference element to each physical element of the mesh to evaluate the expressions of the finite-element matrices : this allows to save a lot in terms of computational efficiency and memory consumption. Indeed, in the linear case, the finite element matrices for the physical elements are simply multiples of the precalculated matrices of the reference element, since the Jacobian of the corresponding transformation is a constant. In a curvilinear setting, the reference element is mapped to the physical element *via* a quadratic form, thus allowing a quadratic representation of boundaries. Therefore, the Jacobian of this transformation is no longer a constant, and the matrices have to be evaluated by means of numerical integration, and stored for each physical curved tetrahedron. Efficient quadrature and cubature rules can be easily found up to sufficient order to our purposes.

A DGTD scheme accouting for curved elements was formulated and implemented in the framework of Maxwell's equations, using upwind numerical fluxes. A validation step was conducted to verify the stability and accuracy of the method. Realistic situations related to the nanophotonics field were then considered that demonstrate the potential of the approach, such as the plasmonic resonance of gold nanosphere dimers (see figure 1).



(a) Rectilinear $\mathbb{P}_4$ computation

(b) Curvilinear $\mathbb{P}_4$ computation

Figure 1: **Near-field visualization of the electric field Fourier transform for a gold nanosphere dimer.** The computation is conducted with $\mathbb{P}_4$ approximation, for both rectilinear and curvilinear meshes. The field values are normalized to 1 in both cases.

Light propagation simulation in complex systems: from semi-continuous metallic films to clusters of disordered nanoparticles

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May 31, 2016

Abstract

The study of light propagation in complex structures has become a very active field of research in the past twenty years because of nice applications in imaging [Seb01] and potentially in the control of light-matter interaction. To validate the theoretical models derived for these kinds of systems and in addition to experiments, there is a strong need in quantitative numerical simulations. In this talk, I will detail two numerical methods we have intensively used in various physical problems involving light propagation in disordered (nano-)structures: the moment or volume integral method [Har92] and the coupled dipoles method [Lax52]. For both I will focus on the advantages and limitations in term of accuracy and requested computing resources. I will also give two examples of physical systems we have considered using these numerical methods and present the associated results: first I will talk about the near-field optics of semi-continuous metallic films [CPC13] and second, I will detail some nice features of light propagation in disordered clouds of dipolar nanoparticles [FCPC15, LPC15].

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Modal analysis of V-groove plasmonic waveguides: A comparison of different formulations.

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Summary

Among the diverse Surface Plasmon Polariton waveguide type, V-shaped dielectric gap waveguides achieve subwavelength confinement and low propagation losses. Numerical modelling of these wave-guides require advanced numerical methods with high efficiency and accuracy especially when the wave-guides include materials with negative permittivity. The problem comes from the difficulty to enforce accurately boundary conditions with complicated geometries which in turn determines the overall effectiveness of the solver. In linear numerical methods, the wave-guide cross section is discretized and a linear matrix eigenvalue problem is derived by using the method of Moments. The effectiveness of any numerical modal method is linked with the mesh that is used to describe the geometry and by the expansion and test basis chosen in the computation. Matched coordinates allow to make the boundary of the wave-guide coincide with surfaces of coordinates which facilitates the writing of boundary conditions. Adaptive spatial resolution have also shown to be a powerful tool to improve the effectiveness of various numerical modal methods. In addition to the above geometrical aspects, using sub-domain basis like polynomials or splines allow to enforce boundary conditions rigorously.

In our presentation, we shall derive different theoretical formulations of the modal method and describe their implementation in various basis. V-groove plasmonic waveguides will be used as an illustrative example.

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Nanophotonics for Solar Cells: current status and future challenges

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Abstract

Reducing the thickness of solar cells is a major challenge in photovoltaics. It is a key toward cost reduction and efficiency improvments, but it requires novel photon management strategies. Conventional light trapping in solar cells is based on (incoherent) lambertian light scattering achieved with rough interfaces, and result in longer optical path length. However, this approach is not suitable for thin-film solar cells with thicknesses below 1 μm.

We have proposed a new paradigm for light trapping. It is based on (coherent) multi-resonant absorption in periodically nanostructured absorbers. Broadband absorption is achieved with a series of overlapping resonant modes in the critical coupling regime. We have demonstrated that this multi-resonant absorption limit exceeds the conventional lambertian limit for any absorber thickness, and could allow a drastic reduction of the absorber thickness in thin-film photovoltaics. However, this approach requires a very accurate design of periodical nanostructures and is very demanding from the numerical and experimental point of view.

In this contribution, we will first introduce the motivations for the development of novel light-trapping strategies, and we will describe the theoretical basis of multi-resonant light trapping. Then, we will provide numerical and experimental examples of multi-resonant absorption in ultra-thin semiconductor layers, and we will draw an overview of current state-of-the-art.

Finally, we will discuss the main numerical challenges that should be addressed to reach the multi-resonant absorption limit: increase the geometrical degrees of freedom, break symmetries, and specific issues for silicon (Si) solar cells related to multi-scale computation (nanostructures combined with periods and/or thicknesses much larger than the wavelength).

Nonlinear optical phenomena whithin the Discontinuous Galerkin Time Domain scheme

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Abstract

The nonlinear interaction of light and matter leads to a broad range of exciting optical phenomena, which depend on and give insight into the structure and properties of matter. Within this work, we mainly focus on second-order nonlinear effects in nanoplasmonic structures, which involve wave-mixing-phenomena such as Second-Harmonic Generation (SHG) and Sum-Frequency Generation (SFG). In addition, we also consider the third-order non-resonant Raman Scattering (RS) in dielectrics. We treat these nonlinear processes in a purely classical manner and solve the Maxwell equations along with the corresponding nonlinear material equations via the Discontinuous-Galerkin Time-Domain (DGTD) finite element approach [BKN11]. In this approach the material models enter the Maxwell curl equations via the current densities. Regarding the second-order response in nanoplasmonic structures, we use a hydrodynamic model in combination with a perturbative approach [HMM+16], whereas we use a polarization current density within the Born-Oppenheimer approximation [BW89, GT06] for the Raman active dielectrics.

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Nonlocal and nonlinear plasmonics in nanowire dimers

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Abstract

We study plasmonic modes in cylindrical nanowire dimer systems by means of a fully nonlinear and nonlocal hydrodynamic Drude model which was implemented via a discontinuous Galerkin time-domain method [HMW+16, HMM+16]. In order to classify the modes which pertain to such systems, we solve the electrostatic problem using a conformal transformation. In our simulations, the system is first excited by broad band Gaussian light pulses under different angles in order to allow for the excitation of all available modes (which may be symmetry-forbidden for certain angles). We observe a strong influence of nonlocality on the linear scattering and absorption spectra and are able to fit all observed modes into the aforementioned classification scheme. To probe the nonlinear behavior, we excite the system with spectrally sharp pulses and record the second harmonic signal. We find that for different angles of incidence, modes which are symmetry-suppressed in the linear spectra can be excited through second-order nonlinear processes.

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Discontinuous Galerkin Time Domain Methods for Nonlocal Dispersion Models and Electron Beam Modeling in the Context of Nanoplasmonics

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June 10, 2016

Abstract

This contribution consists of two main parts: non-local dispersion models and the numerical modeling of single electron beams. Both subjects are discussed in the context of computational nanophotonics for metallic nano-structures.

Non-local dispersion models take into account the non-local nature of mutual electron interaction in the electron gas for metallic nano-structures. Contrary to local models (Drude, Drude-Lorentz,...), non-local models allow additional solutions such as electron density waves that can travel inside the metal bulk [SN16, JAP11]. However, these effects only appear for structures at the size of 2 nm to 25 nm.

Electron beams traveling in the vicinity or inside metallic nano structures excite plasmons. Microscopy techniques like Electron Energy Loss Spectroscopy (EELS) and Cathodoluminescence (CL) are examples of applications. These technologies exploit the electron-plasmon interaction in order to measure plasmonic mode patterns [GdA10].

Both physical aspects are numerically modeled in 3D discontinuous Galerkin time domain (DGTD) framework in order to provide a deeper understanding of the underlying physics.

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Numerical study of the plasmonic effect and optical behavior of Ag@SiO 2 core-shell nanospheres incorporated in organic solar cell

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September 1, 2016

Abstract

One of the approaches used to enhance the performance of organic solar cells (OSCs) is to increase the light absorption in the active layer by employing nano- or micro-structured features that trap light at specific wavelengths or by using the localized surface plasmon resonance (LSPR) effect of metal nanoparticles (NPs) [1]. In spite of a few successful results on direct mixing of metal NPs in the active layer for effective light-trapping, there is often a concern about poor device performance caused by exciton quenching [2]. Futhermore, the metallic NPs are easily oxidized under ambient conditions [3]. To eliminate both the oxidation and the concern about exciton quenching by avoiding direct contact between Ag and the active layer, a possible solution is to protect the metallic cores with dense dielectric shells [2–5]. Another beneficial effect of such core-shell NPs is to prevent shunt currents which could occur in thin film photovoltaic devices due to the possible migration of NPs. In this paper, we numerically study plasmonic solar cells in which a square periodic array of core-shell $Ag@SiO_2$ nanospheres (NSs) are placed on top of the indium tin oxide (ITO) layer (Fig.1) using a 3D-FDTD method. We investigate the influence of various parameters such as the periodicity of the array, the Ag core diameter, the active layer thickness and the shell thickness on the optical performance of the OSC. Our results show that the optimal periodicity of the array of NSs is dependent on the size of Ag core NSs in order to maximize optical absorption in the active layer. A very thin active layer ($< 70nm$) and an ultrathin ($< 5nm$) SiO_2 shell are needed in order to obtain the highest optical absorption enhancement. Strong electric field localization is observed around the plasmonic core-shell nanoparticles as a result of localized surface plasmon resonance (LSPR) excited by Ag NSs without (Fig.2) and with silica shell (Fig.3). Embedding 50nm $AgNSs$ with 1nm-thick SiO_2 shell thickness on top of ITO leads to an enhanced intrinsic optical absorption in a 40nm-thick P3HT:PCBM active layer by 24.7% relative to that without the NSs.

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Problems encountered when modeling dispersive materials using the FDTD method

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May 25, 2016

Abstract

Although the Finite-Difference Time Domain (FDTD) method is well established and widely used for spectroscopic studies, the description of dispersive media is still the subject of many difficulties. They mostly arise from the fact that analytical laws of dispersion are required, and the parameters of these laws have to be optimized for the range of frequencies of interest [BS01, SB06]. A well known methods specifically developed for the the study of dispersive media is the recursive convolution method [KL93]. Typical laws used for the description of dispersive materials are the Debye model, the Drude model, the Lorentz model, or any linear combination of these models. Examples of studies made using such combinations with the above methods have been published for gold [VGM$^+$05] (Drude and Lorentz) or silver [LG05] (Drude and two Lorentz poles).

A new analytical model called the Critical Point (CP) model was then introduced for the description of gold in the 200-1000 nm wavelength range [ERM06]. It was shown that this model could be implemented with only few modifications to existing codes already written to take the Lorentz model into account [Via07]. Moreover, when used as a correction of the Drude model, it may allow a better description of the permittivity than the Drude-Lorentz model, over a wider range of wavelengths, for several metals [VL07][VL08]. This opens the possibility to perform spectroscopic studies for metallic structures over a wide spectrum without the need of too many additional lorentzian terms, thus keeping the FDTD memory requirements as low as possible. It also makes the study of bimetallic structures easier, as the respective permittivities of both metals can be described on the same range of wavelengths, still with a lower memory footprint as previously [VLDL11].

A key point that is nevertheless barely considered is the stability of the model of dispersion. A good fit of the permittivity does not mean that the set of parameters obtained will be adapted to the FDTD algorithm. We will see that it is possible to define a necessary condition, but further tests are required before the stability can be assessed.

Acknowledgement

Most of the work presented here was made in close collaboration with Loïc Le Cunff (UTT) and Thierry Laroche (Frec‖n‖sys).

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Quantum hydrodynamic theory and finite element method for multi-scale plasmonics

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Abstract

The quantum hydrodynamic theory[TSK+15, Yan15, CDS16] is a promising method for describing microscopic details of macroscopic systems, allowing effects occurring at different scales (such as, electron spill-out, tunneling, non-local absorption, retardation effects) to be treated within a single framework. The hydrodynamic equation can be directly obtained from a single particle Kohn-Sham equation that includes the contribution of an external vector potential[Cir16]. This derivation allows to straightforwardly incorporate in the hydrodynamic equation an exchange-correlation viscoelastic term[VK96, VUC97], so that broadening of collective excitation can be taken into account, as well as a correction to the plasmon dispersion. The quantum hydrodynamic model is implemented using a commercial software based on finite element method, with virtually the same computational cost of a standard hydrodynamic description[TRJ+12, RBWM15, CPS13]. The result is an accurate self-consistent and computationally efficient hydrodynamic description of the free electron gas. A very accurate agreement with full quantum calculations is shown.

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Quasi-normal mode computation and its use in photonics

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Abstract

Computing the eigenmodes of an operator corresponding to some physical wave problem provides very useful information: The eigenvalues correspond to the frequencies leading to the strongest responses of the system i.e. resonances and the eigenstates are often an interesting basis to analyse/discretise the problem or even a family of closely related problems.

Here, for the sake of clarity, we consider lossless media, operators are Hermitian, and eigenvalues of bounded problems are real. In the case of photonics and Maxwell's equations, the geometrical domain is often unbounded and Outgoing Wave Conditions (OWC) replace boundary conditions at finite distance. As a consequence, the spectral properties are deeply affected : there are (most of the time) no more eigenmodes and a continuous spectrum (related to the so-called radiation modes) appears. Moreover, 'physical resonances' can be associated to complex frequencies (the imaginary part is associated to the decay rate/quality factor due to the power leakage in the unbounded surroundings) but they are not directly available since they are not strictly speaking eigenvalues. These resonances are called the **quasi-normal modes**. An efficient theoretical and numerical tool to compute them are the Perfectly Matched Layers (PML) that are absorbing layers of finite thickness, surrounding the domain of interest, design to exactly simulate the unboundedness. Corresponding to a complex valued change of coordinates, the PML break the hermiticity of the operator and the effect on the spectrum is to rotate the continuous spectrum in the complex plane and to unveil the resonances associated to the complex frequencies.

In this presentation, we will show how open resonators and open waveguides can be analyzed in practice using FEM modelling associated to PML and complex eigenvalue computation. We will also discuss the possibility of using the eigenmodes to perform efficient computations such as LDOS determination [VZNC14].

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Resonances in frequency dispersive electromagnetic structures: Auxiliary fields and numerical linearization

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Abstract

When dealing with frequency dispersive structures in electromagnetism, the corresponding eigenvalue problem becomes non-linear since the operator at stake depends precisely on the unknown eigenfrequency. This is a major limitation for modal interpretations of physical phenomenons in nanophotonics, where popular structures involve noble metals and semi-conductors whose permittivities exhibit sharp dispersion relations. We propose to use the finite element method to perform the numerical calculation of electromagnetic modes in dispersive and absorptive systems. The dispersion is tackled in two different ways: (i) In the frame of an extension of Maxwells equations where auxiliary fields are added to the electromagnetic field [Tip98, BGD16] and (ii) using non-linear (polynomial) eigenvalue solvers [RCRT16].

These methods are applied to multi-domain cavities and photonic crystals including Drude and Drude-Lorentz metals. Numerical results are compared to analytical solutions for simple cavities and to previous results of the literature for photonic crystals, showing excellent agreement. The advantages of the developed methods lie in the inherent versatility of the finite element method regarding geometries and in sparing the use of the tedious complex poles research algorithm.

Hence, the complex spectrum of resonances of non-Hermitian operators and dissipative systems, like two-dimensional photonic crystals made of absorbing Drude metal, can be investigated in detail. These methods are used to reveal unexpected features of their complex band structure.

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Second Harmonic Generation in stitched PPLN waveguides

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Periodically poled nonlinear ferroelectric crystals are widely used for frequency converters and photonic devices. Lithium Niobate ($LiNbO_3$, LN) is one of the best materials for domain engineering due to its large electro-optical and nonlinear-optical coefficients [1]. The ability to combine periodical poling and low-loss waveguides fabrication makes LN a very attractive material for integrated optics [2]. We have presented detailed study of domain structure formation by e-beam irradiation in congruent LN (CLN) containing waveguides produced by the Soft Proton Exchange (SPE) process and poled by e-beam. Using this technique we have produced Periodically Poled LN (PPLN) channel SPE waveguides and we have given an estimation of the nonlinear conversion efficiency [3]. We have created periodic domain structure in SPE channel waveguide with aspect ratio close to 0.4. SHG experiments were done using a TUNICS T100S-HP tunable laser with a fiber amplifier delivering 100 mW within the wavelength range 1535-1570 nm. For 1.5 mm-long periodically structures, we obtained up to 48%W cm^2 normalized nonlinear conversion efficiency. We have created longer domain patterns by joining up to 4×1.5 mm-long structures. However the joints may present stitching errors.

The aim of this communication is to present the spectral results of such composed structures. In the reversible SHG mechanism, it is expected that a phase shift of the order of π corresponding to a damaged stitching, will reverse the gain obtained in the precedent segment, and therefore destroy SHG at resonance. The spectrum obtained by the tunable laser allows us to explore the spectral domain around quasi-phase matching and the originality of our study is to numerically prove that stitching causes splitting of the spectrum into several bumps keeping the total conversion as is experimentally shown. A π phase shift stitching yields zero conversion at QPM but splits the spectrum in two bumps conserving total conversion. A lot of multiple humped spectra have been obtained depending of different phase shift values. We present in the figure the spectrum for a 4×1.5 mm-long structure containing three stitchings with one almost a π shift. The left-hand figure for the experimental spectrum is numerically reproduced in the right-hand figure by simulating the SHG equations.

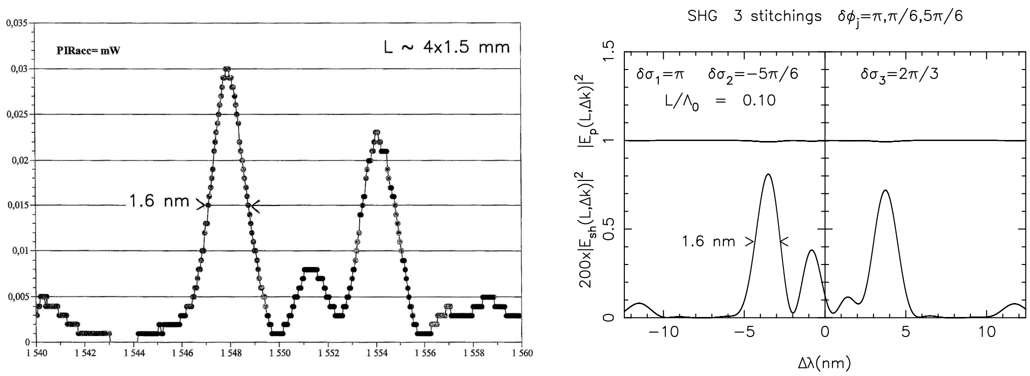

Figure 1: (Left) Experimental SH spectrum: power (μW) vs. fondamental wavelength (nm), and (Right) numerical normalized pump power and 200× normalized SH power vs. $\Delta\lambda = \lambda_p - \lambda_p(QPM)$ for a 4×1.5 mm-long PPLN structure containing three stitchings which almost one exhibiting a phase shift nearby π.

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Simulation d'une cavité à modes de Tamm optiques

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En plaçant une source lumineuse à proximité d'une surface métallique, on excite à l'interface diélectrique (ou vide)/métal des ondes en surface, qui sont dues à l'oscillation couplée de l'onde électromagnétique et des électrons du métal, appelées plasmons polaritons de surface (SPP), de polarisation transverse magnétique [TM] [**1**].

Par ailleurs le confinement d'une onde entre un métal et un miroir de Bragg (Figure 2) engendre à l'interface métal/miroir des ondes qui se propagent à la fois en mode transverse électrique [TE] et en transverse magnétique [TM] [**2**] appelées modes de Tamm optiques. Le fait que les TPPs peuvent être excités directement par incidence normale [3] contrairement aux SPPs constitue un avantage pour le couplage entre source émettrice et rayonnement en champ lointain.

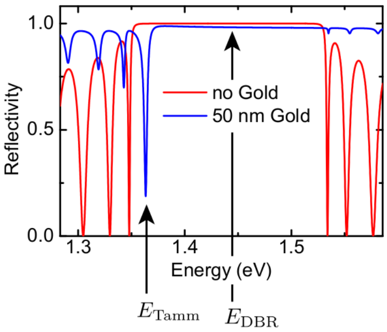

Figure 1: Réflectivité du miroir de Bragg sans (rouge) et avec disque d'or (bleu): mise en évidence de la présence des modes Tamm [**3**]

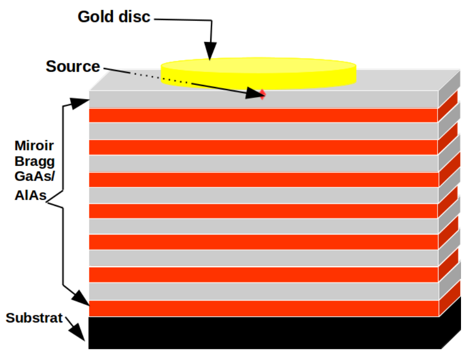

Figure 2: Structure à modes de Tamm optiques

Notre travail se portera sur l'étude d'une structure (Figure 2) constituée d'une source émettrice placée au centre d'un disque métallique d'or de diamètre D= 3 μm au plus et d'épaisseur inférieure à la profondeur de pénétration de l'or à la fréquence choisie et un miroir de Bragg de GaAs/AlAs d'indices ($n_{GaAs} = 3.5$ et $n_{AlAs} = 2.9$) [**2**] constitué de 20 paires de couches.

On utilise pour simuler cette structure le logiciel Meep qui utilise la méthode finite-difference time-domain (FDTD). Le calcul de la réponse de la structure étudiée à une excitation électromagnétique impulsionnelle donne accès aux modes de résonance de la structure. L'objectif de ce travail sera de faire des simulations et une étude expérimentale pour identifier le mécanismes de couplage entre les modes Tamm optiques (à l'interface entre métal et miroir de Bragg) et SPP (interface métal/vide).

De futures études seront consacrées à la directivité et au diagramme de rayonnement, au gain et à la capacité de rayonnement en champ lointain de la structure.

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Simulation of second harmonic generation from photonic nanostructures using the Discontinuous Galerkin Time Domain method

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Abstract

We apply the Discontinuous Galerkin Time Domain (DGTD) method for numerical simulations of the second harmonic generation (SHG) from various metallic nanostructures, in particular arrays of golden split-ring resonators and hybrid metal/dielectric nanoantennas (Fig. 1a) A Maxwell-Vlasov hydrodynamic model is used to decribe the nonlinear effects in the motion of the excited free electrons in a metal. The results are compared with corresponding experimental measurements of the SHG spectra.

The analysis shows that the nonlinear response of plasmonic metamaterials is a complex interplay between the linear and nonlinear optical properties of the individual building blocks, interaction of their near fields in arrays, and lattice interference effects in the far zone. We also show the efficiency of the DGTD method for heavy numerical simulations in particular due to its great parallel scalability. The Maxwell-Vlasov hydrodynamic model was able to qualitatively reproduce SHG spectra measured in all considered experiments. With such a potential, and with possible technical optimization of the numerical scheme like quality mesh generation and multiple time-stepping in a parallel environment, it seems now realistic to develop more sophisticated models, e.g. with rough surfaces of nanostructures and a more detailed description of the nonlinear electron dynamics near the metal surface in the scales smaller than 1 nm for real-sized, hundred-nm, nanostructures.

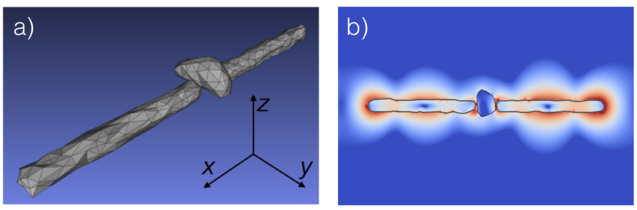

Figure 1: Faceted model of a hybrid metal/dielectric gap antenna with surface roughness and an irregular particle in the gap (a). The log scale colourmap (b) shows non-symmetric distribution of the near field intensity $|E|^2$ at the SHG frequency calculated for a sample structure with surface roughness.

Spatial dispersion in metals : numerical developments and feasible experiments

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Abstract

Drude's model has been extraordinarily successful since its birth in 1900 at describing the optical response of metals. Its is not until very recently[CHM+12] that it has been shown the model could fail - which means it is able to accurately predict the behaviour even of tiny metallic particles in plasmonics. It seems that the limits of Drude's model are found when spatial dispersion kicks in. Spatial dispersion in metals, the fact that it is no longer possible to consider them as regular dielectrics characterized by a (negative) permittivity, arises mainly because of the repulsion that exists between electrons. Models have been developed in the eighties to take this phenomenon into account, but no experiment had been able to back this theory until now[CHM+12].

Now other situations where spatial dispersion has an measurable impact have to be found, to pave the way for future experiments. The sphere coupled to a metallic film has actually a drawback : it involves smaller than 1 nm gaps and other phenomenon, like the spill-out of electrons outside the metal, can not easily be ruled out. Finding new potential experiments however requires to develop new numerical methods that will be able to tackle the problem[BPC+15, DLA+16, SSL+16] and that task.

We have found several structures that would be sensitive to spatial dispersion[MCS13, DTC+16]. All of them have a common point : the excitation of plasmonic guided modes explain their resonances. These guided modes have a very high effective index, and thus an effective wavelength that is close to the mean free path of electrons inside the metals. We will discuss these structures and analyze their physics, as well as the difficulties that might arise when setting up suitable numerical methods.

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Symmetry breaking with spatial Kerr-type nonlinearity in anisotropic metamaterial plasmonic waveguides

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Abstract

Nonlinear plasmonic slot waveguides (NPSWs) have drawn attention in the last decade due to the strong light confinement in the nonlinear dielectric core ensured by the surrounding metal regions, and to their peculiar nonlinear effects [KZ12]. Its modelling has recently been improved for simple isotropic NPSWs [WR16]. Nevertheless, the experimental observation of symmetry breaking in plasmon-soliton waves in symmetric NPSWs is still lacking due to the too high needed power [WRY16]. In this work, we propose and model new symmetric NPSWs thanks the use of an anisotropic metamaterial core with a positive Kerr-type nonlinearity.

First, we demonstrate that for isotropic nonlinear cores with epsilon-near-zero (ENZ) permittivity the bifurcation threshold of the asymmetric mode (the spatial symmetry breaking induced by the nonlinearity) is not reduced, as it is usually expected from ENZ properties, but increased from GW/m threshold to 100 GW/m one. Second, when highly anisotropic diagonal elliptical, but realistic, core with a transverse ENZ component is considered, the bifurcation threshold is now reduced around the 10 MW/m limit gaining more than two orders of magnitude compared to simple NPSWs. This properties indicates a strong enhancement of the effective nonlinearity. Furthermore, the slope of the dispersion curve of the asymmetric mode stays positive suggesting a stable mode. To get these results, we developed specific methods including FEM based ones in order to compute the nonlinear stationary solutions that propagate in these anisotropic NPSWs. For the semi-analytical model we developed, we also provide a closed analytical formula for the effective nonlinearity.

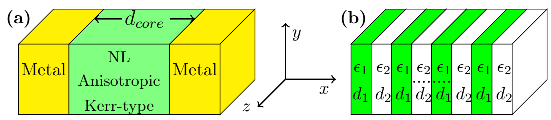

Figure 1: (a) Symmetric NPSW geometry with its metamaterial nonlinear core and the two semi-infinite metal regions. (b) Metamaterial nonlinear core obtained from a stack of two types of layers.

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