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APPLICATION OF THE DISCONTINOUS GALERKIN TIME DOMAIN METHOD TO THE OPTICS OF METALLIC NANOSTRUCTURES

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ABSTRACT. A simulation environment for metallic nanostructures based on the Discontinuous Galerkin Time Domain method is presented. The model is used to compute the linear and nonlinear optical response of split ring resonators and to study physical mechanisms that contribute to second harmonic generation.

1. Introduction

Increasing research activities in the optics of metamaterials, i.e., materials structured at the subwavelength nanoscale, has led to significant progress in the fabrication and experimental analysis. In particular, there is a great interest in the study of plasmon excitations at the surfaces of metallic nanoparticles and at the metal-dielectric interfaces [1]. Resonance interaction of electromagnetic field with electrons in metals result in evanescent plasmon waves confined to the surface of a nanoparticle. In such conditions electron dynamics is governed by linear and nonlinear mechanisms that determine the optical response of the particle.

Due to the small scales of the nanostructures and the evanescent nature of the plasmon waves accurate computer simulations put strict requirements to the numerical methods. Finite Difference Time Domain (FDTD) and Finite Element methods (FEM) are among the most popular that are used in this field [2]. FDTD has proved its efficiency for general problems, however, it is limited by a structured Cartesian spatial discretization. A solution for the geometry that does not conform to rectangular lattice can suffer from a so-called "staircasing" problem and can stay nonconvergent independent of the degree of discretization. FEM operates with unstructured grids and allows flexible description of complex geometries On the other hand, the time domain realization of FEM relies on solving large system of equations and requires many more arithmetic operations per space cell per time step than classical FDTD.

The Discontiuous Galerkin Time Domain (DGTD) method proposed in [3] combines both computational efficiency, explicit time stepping, and the ability to describe complicated geometries without staircasing. In the last years it has been applied to the studies of metallic nanostructures [4,5] as well as large dielectric particles [6]. In this work we use DGTD to simulate the linear and the non-linear optical response of nanoscale metallic split-ring resonators (SRR).

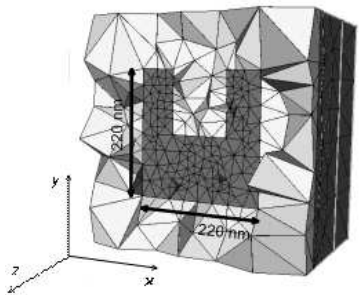

Figure 1. Computational domain cross-section.

2. Numerical method

In DGTD the system of Maxwell equations is solved in the computational domain discretized into a number of conforming elements of arbitrary shape (Figure 1). The electric and magnetic fields are expanded locally, in a single element, in terms of interpolating polynomials. The Galerkin approach [3] is used to construct a set differential equations for time dependent nodal expansion coefficients. Boundary conditions on the interfaces between neighbor elements are introduced and numerical flux terms accounting for field differences on the interfaces are included in the differential equations. Time integration is realized via the 5-stage 4th order Runge-Kutta low storage method. Cyclical representation of an SRR array is realized with periodic boundary conditions in the XY-plane. A perfectly matching layer is applied as an absorbing boundary condition in the Z-direction.

Our DGTD code is based on the publicly available example source written by T. Warburton [7]. The algorithm is effectively parallelized using MPI. Test calculations made on the "Arminius" cluster of the University of Paderborn and the cluster JUROPA of the Juelich Research Center showed excellent scalability at least for up to 1024 CPU cores

To describe a dispersive material we use hydrodynamic treatment, approximating the metal as a free electron gas [8]. To simulate the interaction of the metal with electromagnetic field the following system of equations are solved

$$\mu \frac{\partial \overrightarrow{H}}{\partial t} = -\nabla \times \overrightarrow{E}, \tag{1}$$

$$\varepsilon \frac{\partial \overrightarrow{E}}{\partial t} = -\nabla \times \overrightarrow{H} - \overrightarrow{J}, \tag{2}$$

$$\frac{\partial \overrightarrow{J}}{\partial t} = \frac{n_0 e^2}{m_e} \overrightarrow{E} - \gamma \overrightarrow{J} - \frac{e}{m_e} \left[\left(\nabla \overrightarrow{E} \right) \overrightarrow{E} + \overrightarrow{J} \times \mu \overrightarrow{H} \right] + \frac{1}{n_0 e - \nabla \overrightarrow{E}} \left(\overrightarrow{J} \nabla \right) \overrightarrow{J}. \tag{3}$$

In essence, the current density equation (Eq. 3) includes, correspondingly, the linear Drude term, the nonlinear electric and magnetic parts of the Lorentz force, and a term describing convective acceleration of the electron flow.

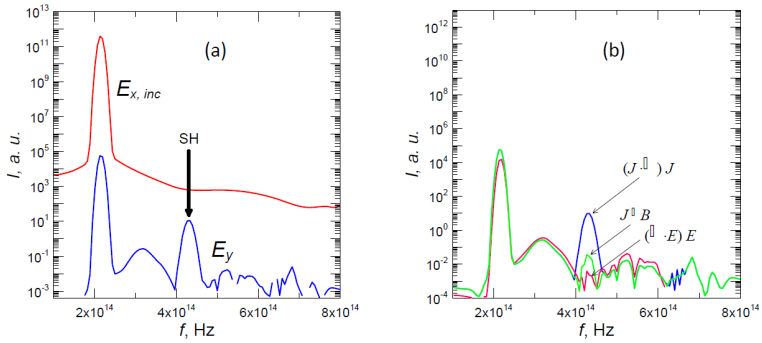

Figure 2. Spectra of two perpendicular polarization components, incident field E_x and transmitted E_y showing fundamental frequency and second harmonic peak (a). Panel (b) shows the E_y component corresponding to the simulations with three nonlinear terms switched independently.

3. Results and discussion

We use a Gaussian pulse with polarization vector directed along the *X* coordinate (E_x) as an excitation driving force. At such orientation of the SRR the solution of the above system of equation results in the higher harmonic generation in the transmission spectra. In particular, an second harmonic (SH) peak appears in the polarization component E_y (Figure 2a) perpendicular to the excitation plane. The peak at fundamental frequency seen in E_y is linear and is due to the imperfect symmetry of the SRR formed in an unstructured mesh. In [9] an experimentally measured SH power conversion efficiency $\eta = |E_{SH}\,(2\omega_0)|^2 \,/\, |E_{inc}\,(\omega_0)|^2$ is reported to be $\eta = 2\times10^{-11}$. Reproducing excitation conditions of the experiment ($E_x = 2\times10^7$ V/m, t =170 fs, λ=1.5 μm) we obtained in our simulation a close value η=4×10^{-11}. Previously, a similar result (η=6.7×10^{-11}) achieved with FDTD method was published in [10].

Numerical simulation allows switching between different terms in the Eq. 3. Figure 2b shows E_y components of transmission corresponding to simulations with each nonlinear term acting independently. One can see that convective acceleration $\left(\overrightarrow{J}\nabla\right)\overrightarrow{J}$ dominates in the SH generation contributing around 90% of total energy.

The intensity of the SH is proportional to the square of the intensity of the excitation pulse which is in agreement with theory. We found that pure DGTD scheme coupled with the current density equation remains stable for the excitation electric field amplitudes up to approximately 5×10^8 V/m. Presence of nonlinearity results in numerical instabilities for stronger fields. The "convective" term $\left(\overrightarrow{J}\cdot\nabla\right)\overrightarrow{J}$ plays here also the main role. The Lorentz force terms appear to be less instable and their instability can be compensated by application of exponential filtering of the solution which introduces artificial energy dissipation in the system [3]. The "convective" term requires a stronger stabilization approach such as involving implicit steps in the DGTD scheme [3,11].

4. Conclusion

From the results of our simulations we can conclude the following.
1. Applied to a nonlinear problem the DGTD method shows numerical stability in the range of field amplitudes that are used in experiments.
2. The strength of the SH signal is close to that measured in experiments. The contribution of the convective acceleration term dominates in the SH peak.

Acknowledgments

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References

[1] W.L. Barnes, A. Dereux, and T.W. Ebbesen, Surface plasmon subwavelength optics, Nature, 424, 824-830, 2003.
[2] A. Taflove, editor. Advances in computational electrodynamics: the finite-difference time-domain method. Boston:Artech House, 1998.
[3] J. S. Hesthaven and T. Warburton. Nodal Discontinuous Galerkin Methods: Algorithms, Analysis, and Applications. Springer Texts in Applied Mathematics 54. Springer Verlag, New York, 2008.
[4] J. Niegemann, W. Pernice and K. Busch, Simulation of optical resonators using DGTD and FDTD, Journal of Optics A: Pure and Applied Optics 11, 114015, 2009.
[5] K. Stannigel, M. Knig, J. Niegemann and K. Busch, Discontinuous Galerkin time-domain computations of metallic nanostructures, Optics Express 17, 14934-14947, 2009.
[6] G. Tang, R. L. Panetta, and P. Yang, Application of a discontinuous Galerkin time domain method to simulation of optical properties of dielectric particles, Applied Optics, Vol. 49, 15,2827-2840, 2010.
[7] http://www.nudg.org
[8] J. D. Jackson. Classical Electrodynamics. New York: John Wiley & Sons, 1998.
[9] M. W. Klein, M. Wegener, N. Feth, and S. Linden, Experiments on second- and third-harmonic generation from magnetic metamaterials, Opt. Express 15, 5238-5247, 2007.
[10] Y. Zeng, W. Hoyer, J. Liu, S. W. Koch, and J. V. Moloney, Classical theory for second-harmonic generation from metallic nanoparticles, Phys. Rev. B 79, 235109, 2009.
[11] V. Doleana, H. Fahsa, L. Fezouia, and S. Lanteria, Locally implicit discontinuous Galerkin method for time domain electromagnetic, Journal of Computational Physics, 229, 512-526, 2010.

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