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

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Abstract. A simulation environment for metallic nanostructures based on the Discon-
tinuous 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 mecha-
nisms 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 experi-
mental 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. Fi-
nite 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 discretiza-
tion. 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 Discontinuous Galerkin Time Domain (DGTD) method proposed in [3] combines
both computational efficiency, explicit time stepping, and the ability to describe compi-
lcated 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).
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

\[ \mu \frac{\partial \vec{H}}{\partial t} = -\nabla \times \vec{E}, \]  
\[ \varepsilon \frac{\partial \vec{E}}{\partial t} = -\nabla \times \vec{H} - \vec{J}, \]  
\[ \frac{\partial \vec{J}}{\partial t} = n_0 e^2 \frac{\vec{E}}{m_e} - \gamma \vec{J} - \frac{e}{m_e} \left[ \left( \nabla \vec{E} \right) \vec{E} + \vec{J} \times \mu \vec{H} \right] + \frac{1}{n_0 e - \nabla \vec{E}} \left( \vec{J} \nabla \right) \vec{J}. \] (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.
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 $\eta = \frac{|E_{SH}(2\omega_0)|^2}{|E_{inc}(\omega_0)|^2}$ is reported to be $\eta = 2 \times 10^{-11}$. Reproducing excitation conditions of the experiment ($E_x = 2 \times 10^7$ V/m, $t = 170$ fs, $\lambda = 1.5$ µm) we obtained in our simulation a close value $\eta = 4 \times 10^{-11}$. Previously, a similar result ($\eta = 6.7 \times 10^{-11}$) 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 $\frac{\mathbf{J} \cdot \nabla \mathbf{J}}{\nabla \mathbf{J}}$ 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 $5 \times 10^8$ V/m. Presence of nonlinearity results in numerical instabilities for stronger fields. The “convective” term $\frac{\mathbf{J} \cdot \nabla \mathbf{J}}{\nabla \mathbf{J}}$ 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.

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References


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