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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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Abstract— We present recent advancements of the development of our DGTD solvers for computational nanophotonics, particularly for metallic nanostructures irradiated by laser pulses or electron beams. By this means, we firstly discuss the numerical treatment of a nonlocal dispersion model for the electron gas which is necessary for structures in the regime of 2 nm to 25 nm. Subsequently, we deal with the modeling of electron beams in 3D simulations for e.g. electron energy loss spectroscopy or cathodoluminescence.

1. INTRODUCTION

The relatively new field of nanophotonics has gained significant importance in the last twenty years. Mainly due to technological advancements on the fabrication side that do now allow the controlled manufacturing of detailed nanostructures for photonic experiments and applications.

Computational nanophotonics is mainly concerned with the accurate modeling of the appearing physical effects in the frequency range of interest and the subsequent solution of the modeling equations. This allows access to detailed understanding of microscopic effects which are fairly often extremely hard to obtain via measurements. Hence, appropriate physical and mathematical models allow systematic optimization, uncertainty quantification, and many other kinds of studies that can be performed at relatively low costs compared to experiments.

Our here presented contribution is the continuation of the presented work in [1]. For the considered geometry and frequency regime, we model electromagnetics by macroscopic Maxwell's equations with additional material equations for the electron gas of the metal structure. Depending on the geometrical size different models have to be considered. We present recent results of time domain simulations of a nonlocal dispersion (also known as nonlocal Drude) model for structures in the regime of approx. 2 nm to 25 nm. The second part of this work deals with the modeling of electron beams for structures in the regime of approx. 20 nm to 500 nm where local dispersion (e.g. Drude, Drude-Lorentz) models are appropriate. In order to efficiently and precisely solve the above-mentioned equations we use a special time domain Finite Element (FE) method. This method is referred to as Discontinous Galerkin (DG) method. The DG method is easily parallelizable, allows local mesh refinement, conforming meshes, curvilinear elements, etc. and can thus precisely handle large structures in reasonable computational times on modern cluster computers.

2. DISCONTINOUS GALERKIN TIME DOMAIN METHOD

The DG Time Domain (DGTD) method is based on a local FE formulation with particular basis functions [2]. This leads to discontinuous solutions in contrast to classical FE methods. Due to the local formulation of DGTD methods only local mass matrices are inverted which yields a significant advantage by means of computational efficiency in comparison to continuous FE methods. Hence, DGTD methods can combine high order basis functions with explicit time stepping and unstructured meshes where the latter is particularly important for complex geometries.

3. NONLOCAL DISPERSION MODEL

Nonlocal dispersion models model the nonlocal nature, i.e. mutual electron interaction in the electron gas for metallic nanostructures. In contrast to local models (Drude, Drude-Lorentz,...), nonlocal models take the microscopic electron interaction directly into account and allow additional solutions by means of electron density waves that can travel inside the bulk. [4, 3] The underlying equa-

Figure 1: Fourier transformed field plot of $|\mathbf{E}|$ at $\omega = 1.1963 \, \omega_\mathrm{p}$. The left plot shows the bulk plasmon mode for an single infinitely long nanowire and the right plot two coupled wires. The coupling of the two wires in terms of the mode pattern is obvious.

tions are:

$$\nabla \times \mathbf{H} = \partial_t \mathbf{D}, \qquad\qquad \partial_t \mathbf{D} = \varepsilon_0 \varepsilon_\infty \partial_t \mathbf{E} + \mathbf{J},$$

$$\tag{1}$$

$$\nabla \times \mathbf{E} = -\mu_0 \partial_t \mathbf{H}, \qquad \omega_\mathrm{p}^2 \varepsilon_0 \partial_t \mathbf{E} = \partial_{tt} \mathbf{J} + \gamma \partial_t \mathbf{J} - \beta^2 \nabla(\nabla \cdot \mathbf{J}), \tag{2}$$

where (2) is a linearized nonlocal Drude model. Here, $\mathbf{H}$, $\mathbf{D}$, $\mathbf{E}$, $\mathbf{J}$, μ_0, ε_0, ε_∞, ω_p, γ, and β respectively are the magnetic field, electric displacement, electric field, polarization current, vacuum permeability, vacuum permittivity, relative permittivity at infinite frequencies, plasma frequency, damping constant, and the quantum parameter.

We have successfully implemented equations (1) and (2) in our DG time domain framework. Figure 1 shows the electric field distribution for a single and coupled infinitely long nanowire.

4. ELECTRON BEAM MODELING

The second part of our contribution addresses the modeling of electron beams in the context of nanoplasmonics. Electron beams traveling in the vicinity or even penetrating plasmonic structure excite plasmons. Microscopy techniques like Electron Energy Loss Spectroscopy (EELS) and Cathodoluminescence (CL) exploit this effect in order to measure/map plasmonic mode patterns [5]. We have recently implemented electron beams and the modeling of EELS as well as CL into our DG time domain framework. First simulation results will be presented.

ACKNOWLEDGMENT

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