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A hybridizable discontinuous Galerkin method for computing nonlocal electromagnetic effects in three-dimensional metallic nanostructures

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ABSTRACT

The interaction of light with metallic nanostructures produces a collective excitation of electrons at the metal surface, also known as surface plasmons. These collective excitations lead to resonances that enable the confinement of light in deep-subwavelength regions, thereby leading to large near-field enhancements. The simulation of plasmon resonances presents notable challenges. From the modeling perspective, the realistic behavior of conduction-band electrons in metallic nanostructures is not captured by Maxwell's equations, thus requiring additional modeling. From the simulation perspective, the disparity in length scales stemming from the extreme field localization demands efficient and accurate numerical methods.

In this paper, we develop the hybridizable discontinuous Galerkin (HDG) method to solve Maxwell's equations augmented with the hydrodynamic model for the conduction-band electrons in noble metals. This method enables the efficient simulation of plasmonic nanostructures while accounting for the nonlocal interactions between electrons and the incident light. We introduce a novel postprocessing scheme to recover superconvergent solutions and demonstrate the convergence of the proposed HDG method for the simulation of a 2D gold nanowire and a 3D periodic annular nanogap structure. The results of the hydrodynamic model are compared to those of a simplified local response model, showing that differences between them can be significant at the nanoscale.

1. Introduction

The field of plasmonics [38,50] studies the collective excitation of conduction-band electrons in metallic nanostructures. These excitations, or plasmon resonances, enable the confinement of light in lengths several orders of magnitude smaller than the wavelength of light, leading to enormous near-field enhancements of the incident wave. The excitation of plasmons is magnified near the corners or sharp features of metallic nanoparticles, or within gaps formed by metallic structures at the nanoscale. Moreover, the extreme confinement and enhancement properties provide unparalleled means for the manipulation of light and its interaction with metals, at scales well beyond the diffraction limit. As a result, the field

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of plasmonics has motivated applications for sensing [62], energy harvesting [10], near-field scanning microscopy [47], plasmonic waveguiding and lasing [60].

Plasmonic phenomena are governed by the propagation of electromagnetic waves. These waves propagate through dielectric as well as metallic media, and several models have been proposed to characterize the behavior of metals. The most common approach to simulate plasmonic structures is to solve Maxwell's equations in both the metal and the dielectric, and account for the losses in the metal through a complex permittivity in the metal given by Drude's model [23]. The effect of the complex permittivity in the metal is to quickly dampen the electromagnetic wave away from the interface. This approach assumes the electrons in the valence band are fully detached from the ions, thus only accounting for electron–electron and electron–ion collisions. The Drude model has limitations due to simplifications in the description of the electron motion that appear at nanometer scales, where nonlocal interaction effects between electrons become predominant [25,26,67]. To account for these long-range interactions, the mathematical model must be enhanced. In this work, we consider the hydrodynamic model (HM) for noble metals, first introduced in the 1970s [24], which models the inter-electron coupling by including a hydrodynamic pressure term. The resulting model is solved simultaneously with Maxwell's equations. For noble metal structures with nanometric and subnanometric features, the HM predicts lower field enhancements and resonance blue-shifts, which are in better agreement with experimental data than the results computed with the Drude model [53,64].

The ability to accurately model and simulate electromagnetic wave propagation problems for plasmonic applications requires capabilities that challenge traditional simulation techniques. The problems of interest involve the interaction of long-wavelength electromagnetic waves (μm and mm) with nanometric cavities for potential applications in sensing and spectroscopy. Additionally, plasmonic phenomena are characterized by the extreme confinement and tight localization of fields in nanometer-wide apertures, nanoparticles, nanometric sharp tips, and even atomically thick materials. As a consequence, the discretizations required to attain accurate simulations need to be adaptive (to concentrate the degrees of freedom in the regions of interest) and anisotropic (to properly capture boundary-layer type structures that appear at the interface of metallic nanostructures).

The first and most widely used method for computational electromagnetics is the finite-difference time-domain (FDTD) algorithm [34,63], which discretizes both space and time using Yee's scheme [65]. The main advantage of Yee's scheme is its simplicity and efficiency, due to the use of staggered Cartesian grids and second-order schemes for both space and time. The main limitation of FDTD is their extension to complex geometries with complex features, since Cartesian grids can only approximate these irregular boundaries in a stair-cased manner. The FDTD method has recently been applied to the hydrodynamic model for the simulation of 2D nanoparticles [39].

Finite-volume time-domain (FVTD) methods have also been devised to solve Maxwell's equations, leveraging high-order Godunov schemes to deal with the hyperbolicity of the system [30,40]. The use of high-order Godunov schemes on a single control volume is appealing, as it renders methods that are amenable to mesh refinement and adaptation, in addition to being low dissipative and dispersive. More recently, there has been an effort to fuse these high-order Godunov schemes from FVTD with the staggering techniques from FDTD, resulting in a new generation of FVTD methods [4,5] that are constraint-preserving, high-order accurate, A-stable, and that accommodate significant variations of material properties at media interfaces.

Finite element (FE) methods [32] are popular techniques for wave propagation problems, thanks to their ability to handle heterogeneous media and complex geometries with the use of unstructured grids. The class of face/edge elements introduced by Nédélec [42] have been extensively used to simulate electromagnetic wave propagation, and have been shown to avoid the problem of spurious modes [9] by appropriately choosing the approximation spaces. A commonly used implementation of edge elements for Maxwell's equations is the one provided by the RF Module of Comsol Multiphysics [22], which has been extended to include the hydrodynamic model [15,64]. Additionally, a frequency-domain implementation of the hydrodynamic model based on edge elements has been applied to the numerical simulation of 2D grooves and nanowires [28].

An attractive alternative to edge elements is the class of discontinuous Galerkin (DG) methods [6,21]. These methods approximate each component of the vector solution independently using standard finite element spaces within each discretization element. The solution across elements is discontinuous, and continuity of the flux is enforced weakly across element interfaces. The DG method with explicit time integration was applied to solve the time-domain Maxwell's equations [27], and has been further developed to simulate wave propagation phenomena through metamaterials at the nanoscale [11], as well as for dispersive media [31,35,37] and more recently for 2D dimers using the hydrodynamic model [59]. DG methods face disadvantages when used for practical 3D applications in the frequency domain or in the time domain with implicit time integration, due to the computational burden that arises from nodal duplication at the interfaces. This shortcoming motivated the development of the hybridizable discontinuous Galerkin (HDG) method, first introduced in [18] for elliptic problems, subsequently analyzed in [17,19], and later extended to a wide variety of partial differential equations (PDEs) [43,44]. More specifically, the HDG has proven very effective for acoustics and elastodynamics [45,58] as well as time-harmonic Maxwell's equations in two dimensions [46] and three dimensions [36]. An additional attractive feature of the HDG method is that, unlike other DG methods, it has optimal convergence rates for both the solution and the flux. As a consequence, its flux superconvergence properties can be exploited to devise a local postprocess that increases the convergence rate of the approximate solution by one order.

The main contribution of this paper is a high-order numerical scheme, the HDG method, to simulate the interaction of light with metallic nanostructures by solving the frequency-domain Maxwell's equations coupled with the hydrodynamic