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Spectral Galerkin Boundary Integral Equation Methods for Plasmonic Nano-Structures

Type:	Interdisciplinary project
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Overview

Currently the minituarization of devices provides rapid progress in the field of nanophotonics. While dielectrics and semiconductors are rather well understood, metals provide a rich and often unexpected variety of new phenomena leading to promising applications for optical telecom, integrated optics, chemical and biological sensing. The light illumination of ultra-small silver or gold particles may give rise to strongly localized *Surface Plasmon Polariton* (SPP) resonances, resulting in powerful near-field amplification both inside and outside the particle with amplitudes which might reach several hundred times that of the illumination. Visual effects of this phenomenon were known for several hundreds of years when artisans had started implementing small metallic particles in the stained glass windows and ornamental cups. Currently the extensive study of both *propagating* SPP and *localized* SPP effects including *Wedge Plasmon Polariton* (WPP), *Gap Plasmon Polariton* (GPP) and *Channel Plasmon Polariton* (CPP) forms the major part of nanophotonics called *plasmonics* which experiences phenomenal growth at both the fundamental research and application levels.

Unusual electromagnetic effects and increasing of the device complexity pose new challenges for numerical simulations. Contrary to dielectric resonances, SPPs strongly depend on the nanoparticle geometry, appear and become more pronounced at low-frequencies and are caused mostly by strong dispersion of metals at optical wavelengths. Therefore the features which are much smaller than a wavelength may have a powerful impact on the SPP resonance behavior. Thus the same computational procedure must be capable of coping with strong local near-field amplitude enhancements, dispersion of materials at optical wavelengths, negative permittivity and non-negligible losses, quasi-static effects with a loose coupling of the electric and magnetic fields and large variety of geometrical configurations involving strong coupling of the device components. Moreover, geometry and material properties have to be taken into account precisely without simplifications and approximations. Then the pursuit to get new numerical simulation algorithm is motivated and justified by the need to find a method that is most efficient in dealing with a category of plasmonic device components of current interest.

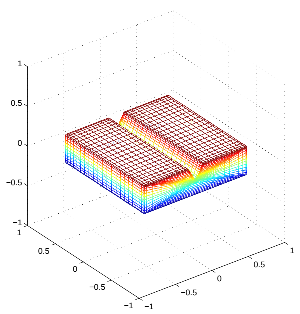
This interdisciplinary project aims to develop efficient numerical algorithms for the fast and accurate numerical simulation of the electromagnetic wave scattering at plasmonic nano–structures. It will include derivation and analysis of suitable boundary integral equations, their spectral Galerkin discretization, developing of efficient preconditioning strategy based on the methods of analytical regularization and the computer implementation of a sophisticated numerical simulation tool, which allows highly accurate numerical solution with low computational cost. This simulation tool will be applicable to all two-dimensional and three-dimensional geometric configurations, which might occur in realistic design of Plasmon Polaritons Enhanced Optical Nanostructures.

The main configurations to be considered are:

1. single (metallic/dielectric) two dimensional and three dimensional particles of arbitrary shape;
2. single coated (metallic/dielectric) particle of arbitrary shape;
3. ensembles of resonantly coupled (metallic/dielectric) particles;
4. single (metallic/dielectric) particle on (dielectric/metallic) substrate;
5. infinite, 1D, 2D, and 3D periodic arrays of (metallic/dielectric) particles;
6. infinite, 1D, 2D, and 3D periodic arrays of (metallic/dielectric) particles in stratified medium.

Details

Unlike in the case of metallic particles considered as perfectly conducting obstacles, the scattering problem for silver/gold nano-particles at optical wavelength leads to a transmission problem for Maxwell's equations. Consider a single-particle plasmonic nano-antenna. It occupies the region of space $\Omega^- \in \mathbb{R}^3$, which is a simply connected bounded domain located in an infinite homogeneous external medium $\Omega^+ = \mathbb{R}^3 \setminus \overline{\Omega^-}$, for simplicity chosen to be vacuum or air. The internal medium Ω^- is characterized by the material parameters $(\varepsilon(\lambda), \mu(\lambda))$ assuming the external excitation by a time-harmonic electromagnetic plane wave with the wavelength λ in free space. *Boundary Integral Equation* (BIE) methods allow a significant advance in solving of such problem due to the presence of linear materials. Deriving the vector Helmholtz equation for electric and magnetic field the resulting transmission problem is reformulated through the representation of the solution as a combination of the curl and double curl of a single layer potential.



The boundary integral equations feature singular and hypersingular integral kernels and give rise to ill-conditioned discrete boundary integral operators. We aim to tackle these operators by means of *analytical regularization* (MAR) involving singularity subtraction and division techniques based on the properties of spherical harmonics. The primary idea is to split the integral operators into a canonical part and a remainder. This step guarantees the efficiency of the algorithm in whole, because the former allows an analytical inversion corresponding to the Mie solution on a sphere. The latter is less challenging to evaluate. The *pole problem* is solved using the properties of spherical harmonics. Finally, the smoothness and periodicity of the remaining kernels permit us to use a Fast Fourier Transform providing the results with high accuracy and reduced complexity of the calculation scheme. Unfortunately, the spectral BIE methods with analytical regularization were mainly developed for acoustic and electromagnetic scattering on perfectly conducting bodies. Moreover the application is restricted to a limited number of shapes for which a global parameterization of the boundary is known. Therefore the main goal of this work is to introduce such a method into nano-optics with the additional flexibility to study bodies with arbitrary shape due to a recently developed strategy.

More precisely, overcome the known shape limitations of spectral methods we conjointly use two techniques:

- *mapping*, that is, paramterizing the boundary $\partial\Omega^-$ over a sphere;
- *patching*, that is, representing the domain Ω^- as a union of several simpler geometries, which are patched across their boundaries by imposing additional requirements on the solution.

For example, the surface $\vec{r}(\eta,\omega)$ of an optical antenna (Figure 1) may be parameterized in a spherical system of coordinates by using the spherical product (1) of the Jordan arc $\Gamma_1 \subset \Gamma$ and the Jordan curve $\Gamma_2 \subset \Gamma$ described by regular mappings $\gamma_1(\eta) : [-\frac{\pi}{2}, \frac{\pi}{2}] \to \mathbb{R}^2$ and $\gamma_2(\omega) : [0,\pi] \to \mathbb{R}^2$ in two orthogonal planes. Here Ω^- is presented as a union of several simpler geometries patched across the boundary by imposing additional requirements on the solution. Note that the surfaces of optical antennas are smooth because at atomic scales "corners" and "edges" are always round. Similar to scattering problems, the application of spectral BIE methods to electromagnetic transmission problems on smooth surfaces provides results with exponential asymptotic convergence rates in terms of number of unknowns.

$$\vec{r}(\eta,\omega) = \gamma_1(\eta) \otimes \gamma_2(\omega), \quad -\frac{\pi}{2} \le \eta \le \frac{\pi}{2}, \quad 0 \le \omega \le 2\pi\ . \tag{1}$$

The project will also target the practically important and numerically challenging study of plasmons propagating along the corrugated metallic surfaces as well as the localized plasmons in the nanoparticles on dielectric substrate. Here we will necessary encounter *non-smooth* material interfaces and corresponding field singularities. While the theory of BIE methods has been already well elaborated for solving of Maxwell equations on Lipschitz domains with constant $\varepsilon, \mu \in \mathbb{R}$, and suitable spectral trial spaces and MAR techniques also have been proposed in two dimensions, the application in the rapidly developing field of nanophotonics has not received much focus comparing with that in the electromagnetic and acoustic community. The theory will be further extended accommodating the realistic functional dependences $\varepsilon(k), \mu(k) \in \mathbb{C}$ of palsmonic materials and broad class of geometrical configutations corresponding to the optical components. Finally, it will be adopted for the developing of fast and efficient numerical simulation algorithm applicable to all optical nanostructures which appear in realistic design of advanced nanophotonic devices.

In addition to the systems of smooth plasmonic nanoparticles and non-smooth plasmonic surfaces the project will involve the study of metalized atomically sharp tips. For the numerical simulation of such a structure the algorithms have to take into account the realistic radii of curvature precisely, which leads to so-called *rounded corner problem.* Considering the corner which is rounded to a scale δ , we have to admit that the singularities are ready to come up when $\delta \to 0$ and the smoothness of the solution in this case is not evident. Some algorithms were already developed for the solving of the boundary value problems on the polygonal domains with slightly perturbed corner with respect to the parameter δ. In our best knowledge the most of them are based on the local transformations in the neighborhood of the perturbed corner, which makes the algorithm of solution in whole domain of investigation more complicate and significantly slow down the numerical simulation process. We aim to tackle this problem by using *smoothed global parameterization* of the polygonal domains which arises from the conformal mapping approach together with patching strategy. The combination of fast convergence of the resulting Fourier series with spherical tensor product gives an opportunity to obtain highly accurate parametric representation of three-dimensional surfaces with arbitrary small δ. Such a parameterization is suitable for the developed on the first stage spectral Galerkin BIE algorithm. When δ tends to 0, the numerical solution tends to those corresponding to the non-smooth particle obtained with the algorithm developed on the second stage.

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