8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

Three-Dimensional Spectral Boundary Integral Equation Analysis of Plasmon Polaritons Enhanced Optical Nanoantenna

*** Lyudmyla N. Illyashenko-Raguin[1], Christian Hafner[2] and Ralf Hiptmair[3]**

[1] D-MATH
Rämistrasse 101, ETH
8092 Zürich, Switzerland
mila.raguin@sam.math.ethz.ch

[2] IFH, D-ITET
Gloriastrasse 35, ETH
8092 Zürich, Switzerland
christian.hafner@ifn.ee.ethz.ch

[3] SAM, D-MATH
Rämistrasse 101, ETH
8092 Zürich, Switzerland
ralf.hiptmair@sam.math.ethz.ch

Key Words: *Spectral Boundary Integral Equation Method, Analytical Regularization, Mapping and Patching, Spherical Product, Plasmon Resonance, Optical Nanoantenna, Channel Plasmon Polariton.*

ABSTRACT

Nanophotonics experiences phenomenal growth at both the fundamental research and application level. Smaller and more complex devices are needed. The interest in their innovation is not slowing down. While dielectrics and semiconductors are rather well understood, metals are promising. Due to strong dispersion at optical wavelengths they exhibit a rich variety of fascinating and often unexpected electromagnetic effects. The light illumination of ultra-small metallic particles may give rise to strongly localized *plasmon resonances* [1]. Such a resonance depends on the material properties, length scale and geometry so strongly that even details, which are much smaller than the wavelength, may have a strong impact on the resonance behavior. Powerful local near-field amplitude enhancements, dispersion of materials, negative permittivity, non-negligible losses and quasi-static effects with a loose coupling of the electric and magnetic fields provide new challenges for numerical simulations [2]. Unlike the case of metallic particles treated as perfectly conducting obstacles in [3], the scattering problem for silver/gold nanoparticles at optical wavelength leads to a transmission problem for Maxwell's equations [1, 4]. Since the energy of plasmon modes is confined to a thin region surrounding material interfaces, it is advantageous to base the analysis on the use of *Boundary Integral Equation* (BIE) methods [2, 3, 4]. While BIE methods based on the boundary approximations by Liptschitz polygon/polyhedron [4] may meet the demands of electromagnetic research, particle shapes in nanophotonics have to be taken into account precisely, describing realistic radii of the curvature. Highly accurate numerical analysis is essential. The goal of this work is to develop an efficient algorithm, the performances of which will be demonstrated on the example of a *Channel Plasmon Polariton* enhanced *optical nanoantenna* [2].
Consider a single-particle nanoantenna located in an infinite homogeneous medium. It occupies the region of space $\Omega^- \subset \mathbb{R}^3$ which is a simply connected bounded domain. Denote the complement as $\Omega^+ = \mathbb{R}^3 \setminus \overline{\Omega^-}$ and the boundary as $\Gamma = \partial\Omega^-$. The 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. For simplicity Ω^+ is chosen to be vacuum or air. Deriving the vector Helmholtz equation for electric and magnetic fields [1] the resulting transmission problem is reformulated presenting the solution as a combination of curl and double curl of

a single layer potential. Resulting surface integral equations feature singular and hypersingular integral kernels which may give rise to ill-conditioned discrete operators. We propose to overcome these difficulties by means of an *analytical regularization* of these operators involving singularity subtraction and division techniques. 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 [1]. 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.

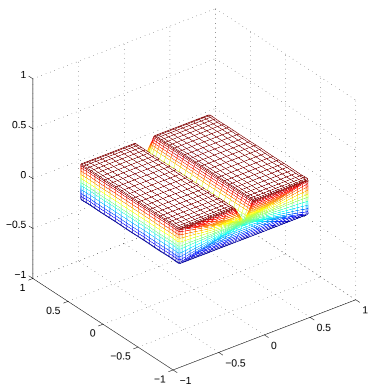

Figure 1: *Parameterization of nanoantenna consisting of a metallic patch with a V-groove for local field enhancement [2]*

This method belongs to the category of *Spectral BIE methods*. Methods of this kind have already been demonstrated to be a powerful approach for acoustic scattering [3] and electromagnetic scattering by perfectly conducting bodies [3]. They provide fast and highly accurate solution with small requirements of memory storage due to smaller matrices compared with those of classical boundary element methods. While the theory of BIE methods has already been well elaborated, the application in the rapidly developing field of nanophotonics has not received much focus compared with that in the electromagnetic community [3, 4]. To our knowledge a spectral BIE method for solving transmission problem on optical antennas was not developed. Moreover, the analytical regularization procedure in [3] was restricted to shapes with known global parameterization over a sphere. The intention of this work is to introduce a spectral BIE method into nanophotonics providing the flexibility to study nanoparticles of *arbitrary shape*. To overcome the shape limitations we propose to develop a parameterization using *mapping*, *patching*, and *spherical products* together.

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 of the Jordan arc $\Gamma_1 \subset \Gamma$ and the Jordan curve $\Gamma_2 \subset \Gamma$ described by regular C^2-smooth 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 [3], 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.

ACKNOWLEGMENTS

We would like to thank Prof. M. Ganesh for providing information about recent advances in Spectral Boundary Integral Equation methods.

REFERENCES

[1] S. Maier. *Plasmonics: fundamentals and applications*, Springer, Berlin, 2007.

[2] Ch. Hafner, X. Cui, A. Bertolace, and R. Vahldieck. “Frequency-domain simulations of optical antenna structures”. *Proc. SPIE.*, Vol. **6617**, 66170E1–12, 2007.

[3] M. Ganesh and I. G. Graham. “A high-order algorithm for obstacle scattering in three dimensions”. *J. Comp. Phys.*, Vol. **198**, 211–242, 2004.

[4] A. Buffa, R. Hiptmair, T. von Petersdorff, C. Schwab. “Boundary element methods for Maxwell transmission problems in Lipschitz domains”. *Numer. Mathem.*, Vol. **95**, 459–485, 2003.