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Fast Integral-Equation Simulation of Plasmonic and Photonic Problems at the Nanoscale

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The great potential of metal/dielectric interfaces and, in particular, metallic nanoparticles (NP) to provide subwavelength confinement, enhancement, and spatiotemporal control of light, has put the field of plasmonics and nanoplasmonics at the forefront of nanotechnology research in the past years. Nevertheless, the optical response of metals is quite different from the high conductivity observed at lower frequencies. Here the response is governed by the plasma-like collective oscillations of the conduction electrons induced by the interaction of electromagnetic radiations [1]. This behavior is responsible for the subwavelength control of light, which in the past years has put the field of nanoplasmonics at the forefront of nanotechnology research.

Research in nanoplasmonics demands the development of efficient and accurate solvers to provide the theoretical background to support the experiments and devise new research opportunities. In this sense, Maxwell's solvers can be safely applied at the nanoscale, and as far as these solvers is concerned, plasmonic nanoparticles can be treated as regular non-magnetic homogeneous dielectrics. Thereby, they are entirely characterized by their dispersive permittivity, despite the underlying physics being quite different of what might be expected for a conventional dielectric. There are several popular methods that are capable of yielding rigorous classical electromagnetic solutions in arbitrary dielectric geometries. In particular, volumetric approaches are increasingly popular in nanotechnology applications, partly due to the availability of commercial software (e.g., COMSOL). Nevertheless, these approaches pose a numerical demand that scales with at least the square of the volume, so they cannot cope with real-life structures spanning several wavelengths in size, as the computational cost becomes impractical even using high computer power capabilities.

A much more computationally efficient approach comprises the use of surface integral equation (SIE) formulations combined with the variational enforcement of the boundary conditions offered by the method of moments (MoM). In this contribution, we present a review of the effort we are making to extend the SIE-MoM, [2] combined with the spectral acceleration of the multilevel fast multipole algorithm (MLFMA) [3], [4] and the domain decomposition (DD) methods [5] for the simulation of realistic large and often multi-scale systems at the nanoscale. Among all the possible applications, we have concerned ourselves especially with biosensing, and particularly with surface enhanced Raman scattering (SERS) based spectroscopy. We will present several examples showing the ability of the SIE approach to accurately predict the SERS spectroscopy in complex, real-life systems. The results will be validated with measurements provided by leading-edge research groups in the context of Raman spectroscopy and plasmonics.

References

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