Modeling of plasmonic, dielectric and hybrid nanostructures with surface integral equations

Parmenion Mavrikakis[1] and Olivier J.F. Martin[1]

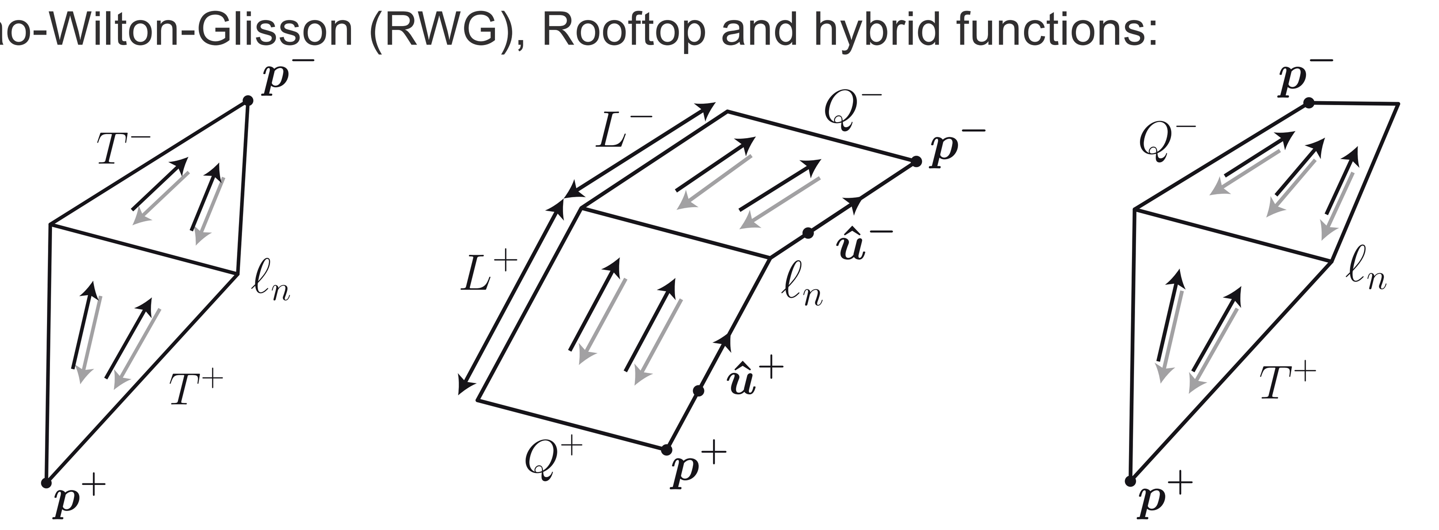
[1]Nanophotonics and Metrology Laboratory, EPFL, CH–1015 Lausanne, Switzerland

1 Introduction

Metasurfaces are usually constructed from meta-atoms, which consist either of plasmonic or dielectric materials. However, recently, hybrid metasurfaces built from meta-atoms that combine both of the aforementioned material categories have emerged. In order to model plasmonic, dielectric and hybrid nanostructures, we resort to the surface integral equation (SIE) method, which is based on the integral form of Maxwell's equations. A finite element approach is used to discretize the equations and we show that different types of elements and basis functions provide specific advantages for the modeling of such systems. In our computational approach, the T-PMCHWT (Poggio, Miller, Chang, Harrington, Wu, and Tsai) formulation is considered [1]. To model experimentally-relevant nanostructures, we employ triangular and quadrilateral elements and treat the Green's function singularity in different ways. This technique is assessed with canonical and more complex geometries that include one or more materials. Furthermore, by using multipoles expansions obtained from the full-field electromagnetic calculations, we present a direct comparison between the accuracy and efficiency of modeling with the aforementioned elements.

2 Basis functions

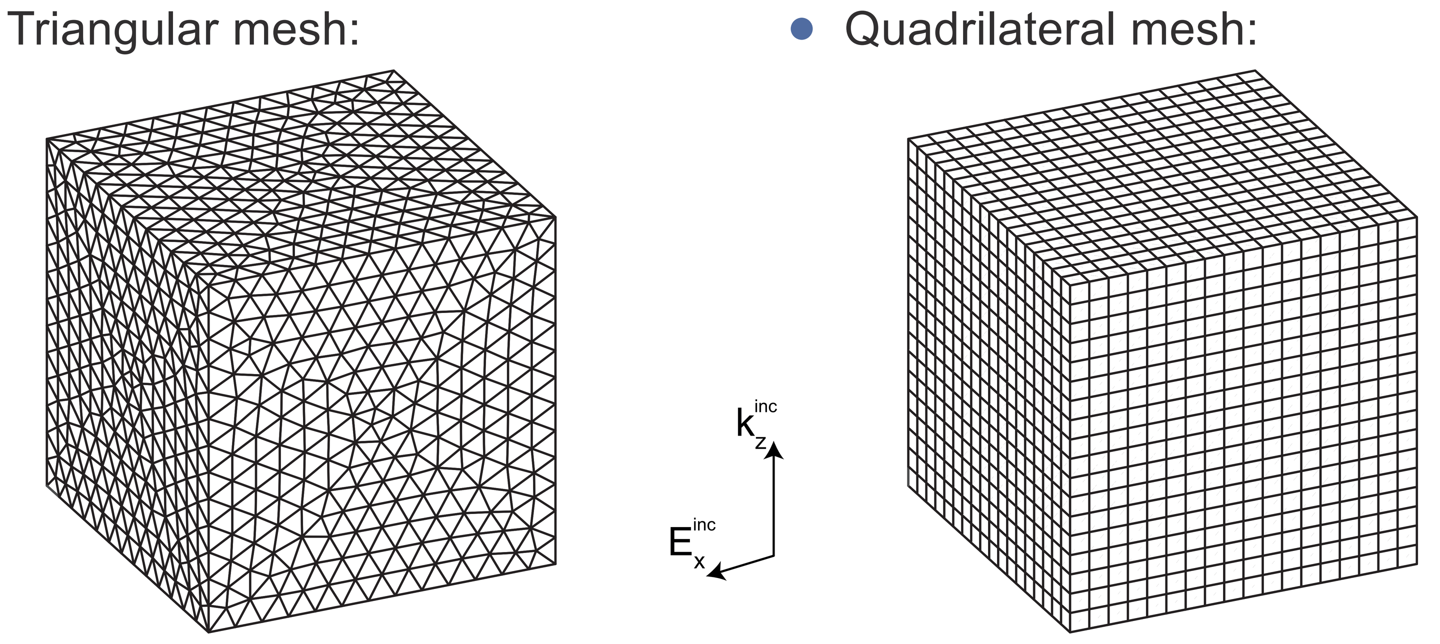
- Rao-Wilton-Glisson (RWG), Rooftop and hybrid functions:



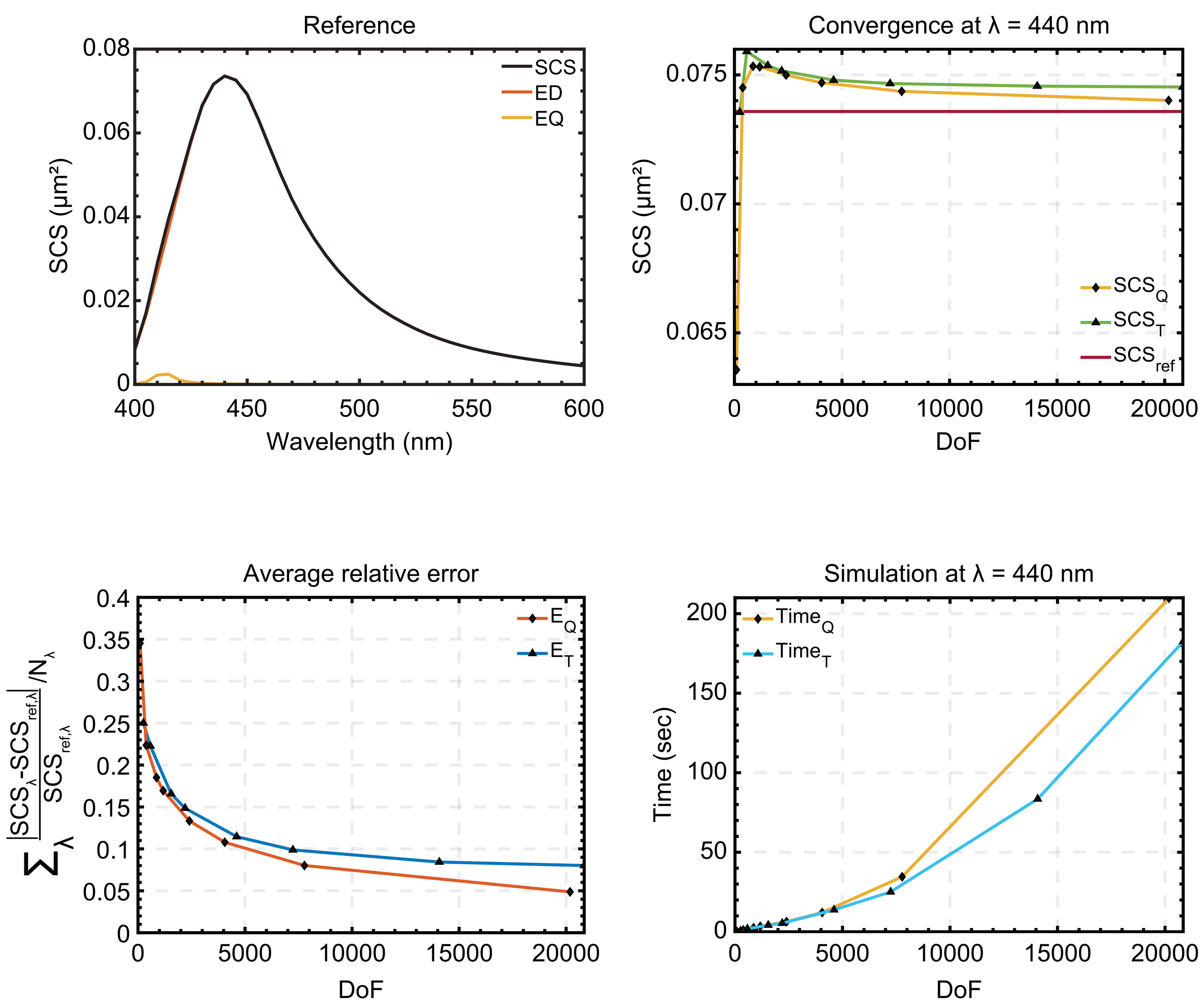
- With triangular elements and RWG functions, it is possible to improve the approximation of non-rectangular surface boundaries or nanoparticles' parts that present geometrical imperfections due to fabrication [2].
- Regarding the discretization of flat surfaces, it can be implemented with quadrilateral elements and rooftop basis functions in order to decrease the number of unknowns in the final system.
- The numerical integration points are chosen carefully to avoid singularities.

3 Silver cube (edge = 75 nm) discretization

- Triangular mesh:
- Quadrilateral mesh:

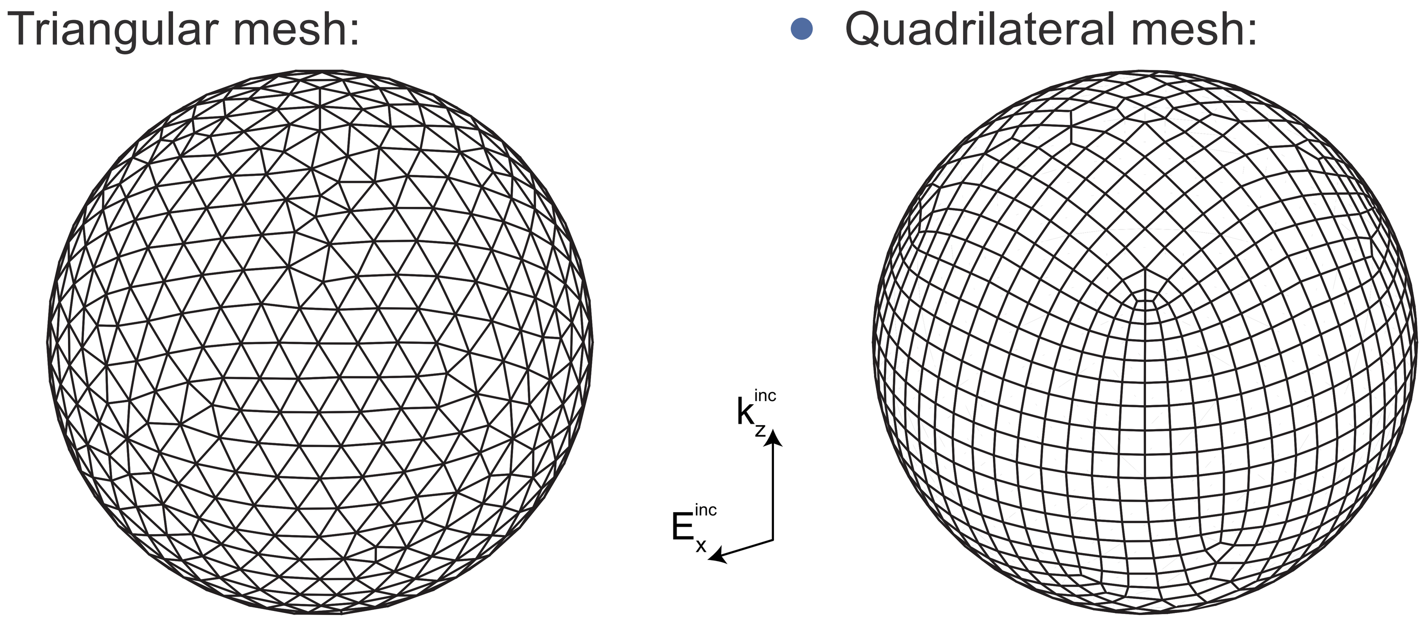


- Illumination with x-polarized plane wave propagating towards z:

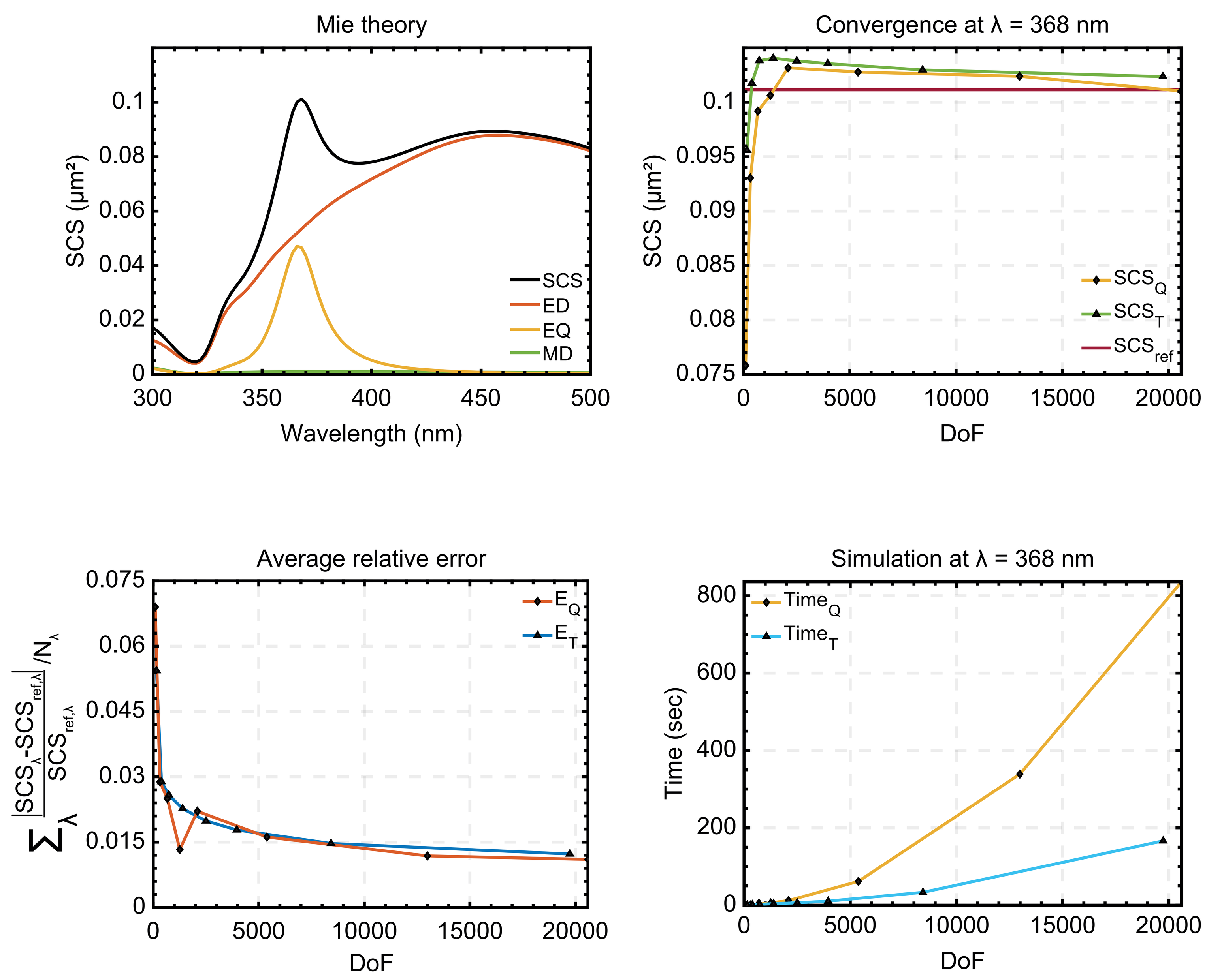


4 Silver sphere (R = 75 nm) discretization

- Triangular mesh:
- Quadrilateral mesh:

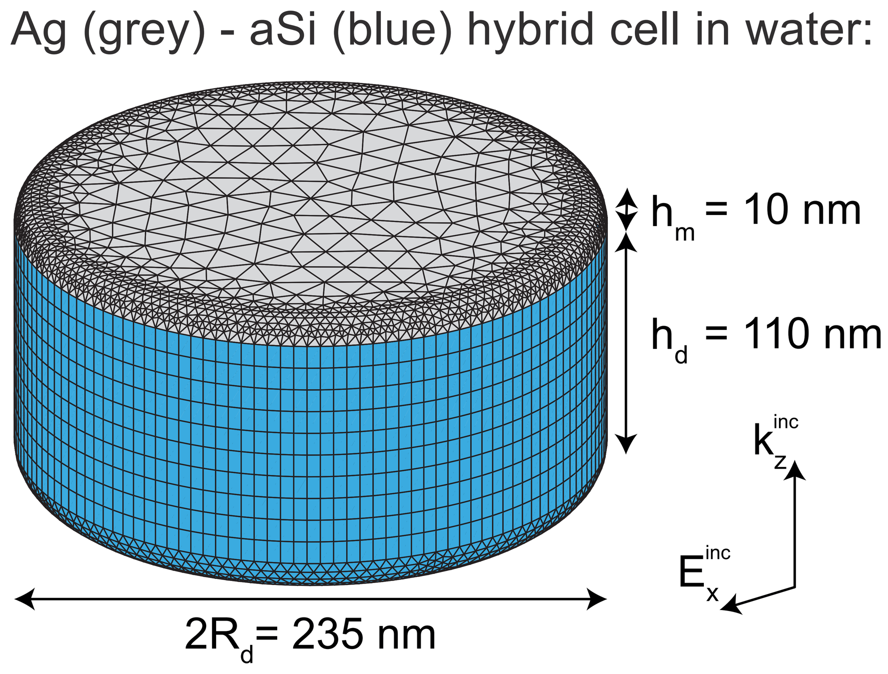


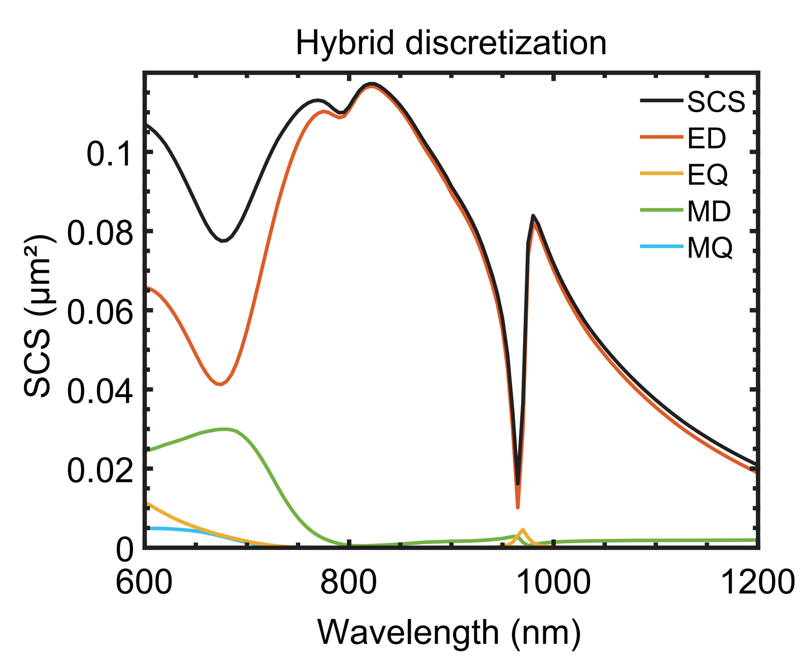
- Illumination with x-polarized plane wave propagating towards z:



5 Nanostructure hybrid discretization

- Ag (grey) - aSi (blue) hybrid cell in water:





- For very dense surface discretization the selection of numerical integration points does not function properly.
- The singularity subtraction technique was applied for both triangular and quadrilateral elements.

6 References

[1] A. M. Kern, O. J. F. Martin, Surface integral formulation for 3D simulations of plasmonic and high permittivity nanostructures, J. Opt. Soc. Am. A 26, 732-740 (2009).

[2] A. Kiselev, J. Kim, and O.J.F. Martin, Mind the gap between theory and experiment, Adventures in Contemporary Electromagnetic Theory, Chap. 21 (T.G. Mackay, A. Lakhtakia Eds.) Springer 2023.

Contact

Parmenion Mavrikakis - EPFL
Email: parmenion.mavrikakis@epfl.ch
Nanophotonics and Metrology Laboratory ~ www.nanophotonics.ch

Swiss National Science Foundation