Full-wave Simulation of Metallic Nanoparticles using Quadrilateral Barycentric Basis Functions

Michael Wei[1] and Weng C. Chew[2]

[1] Department of Electrical and Computer Engineering, University of Illinois, Urbana-Champaign, *mwei5@illinois.edu*

[2] Department of Electrical and Computer Engineering, University of Illinois, Urbana-Champaign, *w-chew@uiuc.edu*

Plasmon resonance in metallic nanoparticles (MNPs) have been used to improve the performance of many nanoscale devices from enhanced photon conversion efficiency in solar cells to increased propagation length in surface plasmon-based circuits. The numerical methods used to simulate the behavior of plasmonic nanoparticles have mostly been FDTD or some approximate method. As technologies using MNPs improve and we move away from proof of concept towards expertly tuned devices, accurate electromagnetic simulation becomes vital for design optimization.

We propose a method for accurate full-wave simulation of plasmonic behavior in MNPs using surface integral equations. A metallic nanoparticle can be accurately modelled as a lossy dielectric. Doing so enables us to examine the fields both outside and inside the MNP. However, upon converting the surface integral into a matrix equation, we encounter the well-known testing problem which is prevalent in surface integrals that use both $\mathcal{L}$ and $\mathcal{K}$ operators. The inaccuracy introduced by poor choice of testing function can be overcome using basis functions that live on a barycentric mesh. An example of this is the Buffa-Christiansen basis function (BCBF). In our approach, we use the quadrilateral barycentric basis function (QBBF) to expand the surface integral equation. Used effectively, QBBF uses far fewer unknowns compared to BCBF. Using polar coordinate transformation, we derive an expression for the integral over the source element which can be used to accurately evaluate diagonal terms in the matrix that is also suitable for highly lossy material at optical frequencies.

To solve the matrix equation iteratively requires a good pre-conditioner. A simple diagonal pre-conditioner proved to be inadequate for reducing the number of iterations in a significant way. The pre-conditioners considered are the Calderón formulation and the newly devised $\mathbf{A} - \Phi$ formulation. Both Calderón and $\mathbf{A} - \Phi$ formulations are block symmetric and provide good convergence not only when the MNP is much smaller than the wavelength but also when the MNP is on the order of a few wavelengths. We explore the performance and accuracy of both formulations over the range of visible light.