Comparative Study of Electromagnetic Field Solvers for the Modeling of Nanoscale Plasmonic Scatterers

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***Abstract* – The nanoscale systems are of great importance in modern science and technology, offering a wide range of possible daily life applications. In order to characterize the electromagnetic (EM) properties of metallic nanotopologies, the commercialized computational tools COMSOL, CST, and Lumerical have been widely used. In this work, the performance of the above tools is compared, through the investigation of the plane wave response of canonical spherical and cubical nanoparticles. It is demonstrated that not all EM field solvers provide an accurate description of the nanoparticle's behavior.**

Keywords - EM field solvers, nanoscale, plasmonics

I. Introduction

The recent advancement in the field of nanotechnology has provided the very capability of miniaturizing classical antennas and scatterers down to the nanoscale, and extending their operating regimes from RF and microwave to optical frequencies. Especially, metallic nanostructures have attracted tremendous interest for many practical applications, ranging from optoelectronics, over information and communication technology, to biomedicine [1–3]. More theoretically, metals may sustain significant losses in the optical frequency range. Since the size of a nanostructure is comparable with the skin depth of the metals, three-dimensional volumetric currents are assumed flowing in the structure. The electron gas of a metal may experience resonant collective motions, which are referred to as plasmons, giving rise to strongly enhanced electromagnetic (EM) fields, confined to sub-wavelength volumes [4].

Concerning the analysis and design of metallic nanotopologies, the following commercially available software tools: COMSOL [5], CST [6], and Lumerical [7] have been widely used. These tools have been established based on different numerical techniques, such as the Finite Element Method (FEM), the Finite Difference Time Domain (FDTD), the Method of Moments (MoM). COMSOL and Lumerical incorporate FEM and FDTD implementations, respectively, and CST provides both FEM and MoM realizations. Nevertheless, the performance of the abovementioned tools, within the framework of modeling the optical response of nanostructures, has not been fully investigated yet.

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The current work reports on a simulation benchmark of four EM field solvers, namely COMSOL, CST (FEM), CST (MoM), and Lumerical. Canonical spherical and cubical nanoparticles are studied, under a plane wave excitation. The analysis is performed through the characterization of the near and far fields of the nanoparticles. For detailed discussion of the associated simulations, we refer the readers to our previous work [8].

This work is organized as follows. Section II provides more details on the studied topology. The observed optical features are also discussed. The numerical results are demonstrated in Section III and explained in Section IV.

II. Analysis Set-up

Two different structures are studied, namely a single nanosphere and a nanocube. Gold and silver are employed as the constituting metals. The associated permittivities in the optical frequency range are described by an experimental material model [9], without considering any nonlocal effects [10,11]. The structures are embedded in a water solution, with a refractive index of 1.34. The nanoparticles are excited by a time-harmonic plane wave with a unit amplitude, polarized in x-direction and propagating along the z-axis.

The following optical features are investigated: 1) the scattering cross section; 2) the E-field intensity at a single spatial point, located 1 nm above the nanoparticle's surface along the x-axis; and 3) the E-plane radiation pattern. In order to evaluate the accuracy of the numerical tools, the analytical Mie theory is used as a reference for the spherical nanoparticle [12]. In the case of the other studied structure, only the comparative study of the employed tools is performed, with COMSOL serving as a numerical reference. More details on the solver environments and simulation parameters are given in [8].

III. Numerical Results

The scattering cross section, the point evaluated E-field intensity, and the E-plane radiation pattern are depicted for a 30-nm-radius gold sphere in Fig. 1. The same features are plotted for a 50-nm-sized silver cube in Fig. 2. The reported results are normalized to the maximum values of the corresponding reference solutions.

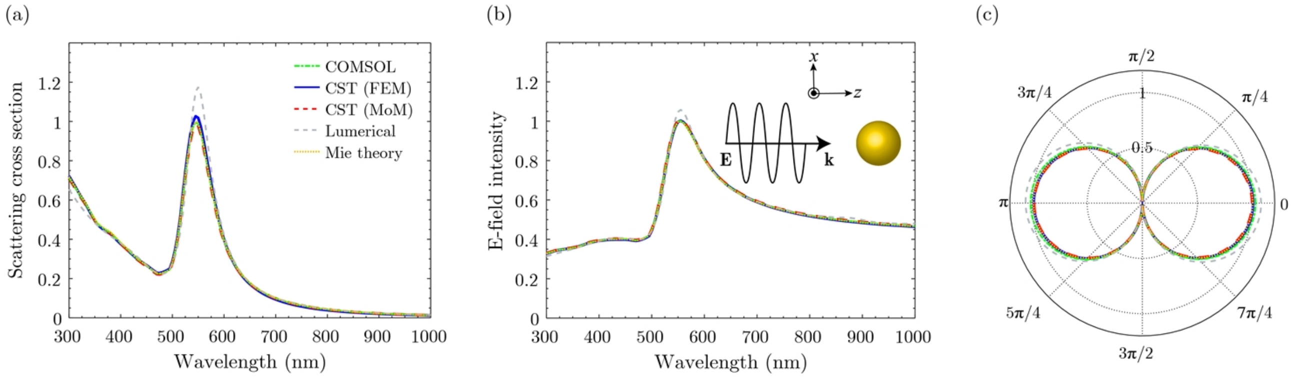

Figure 1. Optical response of a 30-nm-radius gold sphere in water solution: (a) the scattering cross section; (b) the point evaluated E-field intensity; and (c) the E-plane radiation pattern evaluated at 545 nm, corresponding to the maximum of the analytical Mie scattering cross section.

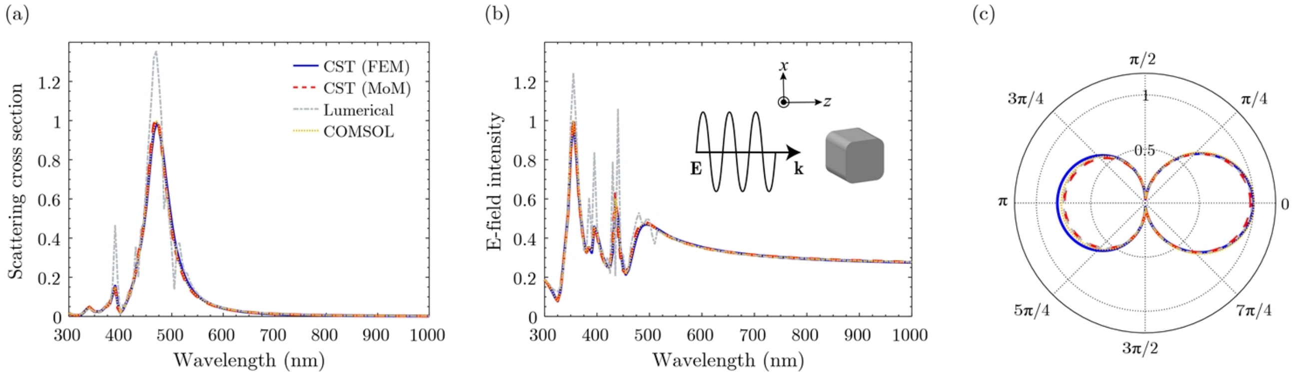

Figure 2. Optical response of a 50-nm-sized silver cube in water solution: (a) the scattering cross section; (b) the point evaluated E-field intensity; and (c) the E-plane radiation pattern evaluated at 355 nm, corresponding to the maximum of the near E-field intensity generated by COMSOL.

IV. Discussion

Considering the results for the spherical nanoparticle, COMSOL, CST (FEM), and CST (MoM) generate an almost perfect agreement with the analytical reference. These tools predict the correct spectrum positions of the near and far field resonances. However, Lumerical introduces a considerable deviation, compared with the other tools. Apart from the noticeable magnitude offset, it yields a 10-nm-redshift of the plasmon resonance in the scattering spectrum, as shown in Fig. 1 (a). The discrepancy is also observed in the near field and radiation pattern, as plotted in Figs. 1 (b) and (c).

As for the other studied structure (i.e. the nanocube), CST (FEM) and CST (MoM) agree closely with the reference solutions generated by COMSOL. In contrast, Lumerical still shows a large discrepancy, producing several striking spurious resonances. For example, the scattering spectrum, illustrated in Fig. 2 (a), reveals three distinguishable anomalous peaks at 430 nm, 490 nm, and 515 nm. This situation is even more concerning for the near field, see Fig. 2 (b), displaying a larger number of spurious components.

Despite conducting more detailed analyses of different simulation parameters, such as the size of calculation domains or meshing steps, Lumerical failed to eliminate the abovementioned artifacts. These issues may be caused by the internal FDTD algorithms, which extract a time domain model for the constitutive properties of the studied materials. Clearly, the same difficulties do not arise for the frequency domain techniques in COMSOL and CST.

V. Conclusion

This work compared the performance of commercially available numerical tools, namely COMSOL, CST, and Lumerical, for the modeling of the optical response of nanostructures. The analysis was performed by investigating the near and far characteristics of isolated spherical and cubical nanoparticles, excited by a plane wave. The nanoparticles were constituted of noble metals, including gold and silver. The following features: the scattering cross section, the point evaluated E-field intensity, and the E-plane radiation pattern, were generated with the tools. The analytical Mie theory was employed as a reference for the spherical shape. It was shown that COMSOL, CST (FEM), and CST (MoM) provide accurate predictions of the nanoparticle's behavior. In contrast, Lumerical performs unreliably and deviates strongly from the other studied EM field solvers. It yields prominent numerical artifacts in the spectrum, especially for the cubical nanoparticle.

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