Self-Consistent Modeling of Coupled Maxwell-Rate Equations with the Finite-Difference Time-Domain Method

P. Mavrikakis[1], **S. Athanasiou**[1] **and O. J. F. Martin**[1]

[1]École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Abstract— The interaction between molecules and plasmonic nanoparticles is central to numerous phenomena in nanophotonics. A comprehensive and accurate description of these interactions requires capturing the time-dependent quantum properties of molecules alongside a classical treatment of the electromagnetic fields. In this work, we present a semi-classical framework based on the finite-difference time-domain (FDTD) method to investigate molecule-plasmon interactions in three dimensions. Our method incorporates several key innovations that distinguish it from conventional techniques. First, it employs the Yee algorithm [1] to calculate electric and magnetic fields, while the molecular rate equations are integrated directly on the Yee grid using a finite-difference scheme. Furthermore, the relevant molecular processes, such as excitation and spontaneous radiative emission, are explicitly influenced over time by the evolution of the electric fields. This approach provides detailed insights into the dynamic interplay between molecular and plasmonic processes. Additionally, the method leverages computational strategies to maintain numerical stability and accuracy across the spatial and temporal scales characteristic of molecule-plasmon systems. Through FDTD simulations in 3D, we compute both near-field and far-field optical responses of the scattering systems, while resolving the time-dependent dynamics of the molecule-plasmon system under various scenarios such as pulsed or electrical excitation. Our approach unveils intricate details about energy exchange processes and the influence of plasmonic fields on molecular behavior. This work establishes a robust computational framework that bridges theoretical and experimental studies, advancing the understanding of molecule-plasmon interactions. By providing novel insights into the temporal and spatial dynamics of molecule-plasmon systems, our approach contributes to the development of innovative nanophotonic design and simulation tools, advancing the frontier of nanophotonics research.

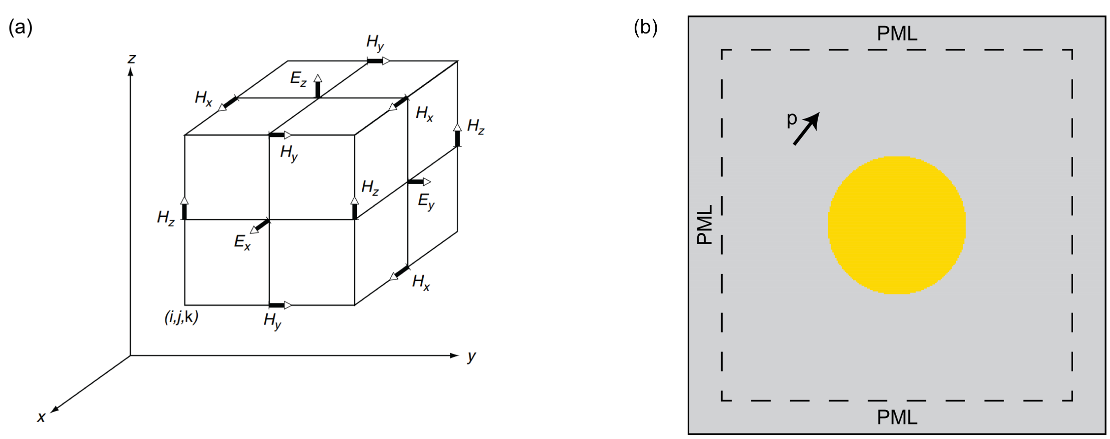

Figure 1: (a) Electric and magnetic field components on a cubic Yee cell [2], and (b) 2D cross section of a molecule (dipole) and plasmonic (gold) nanoparticle 3D geometry.

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