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Electromagnetic Simulations of Metal Nanoparticles and Metal Nanoparticle Assemblies

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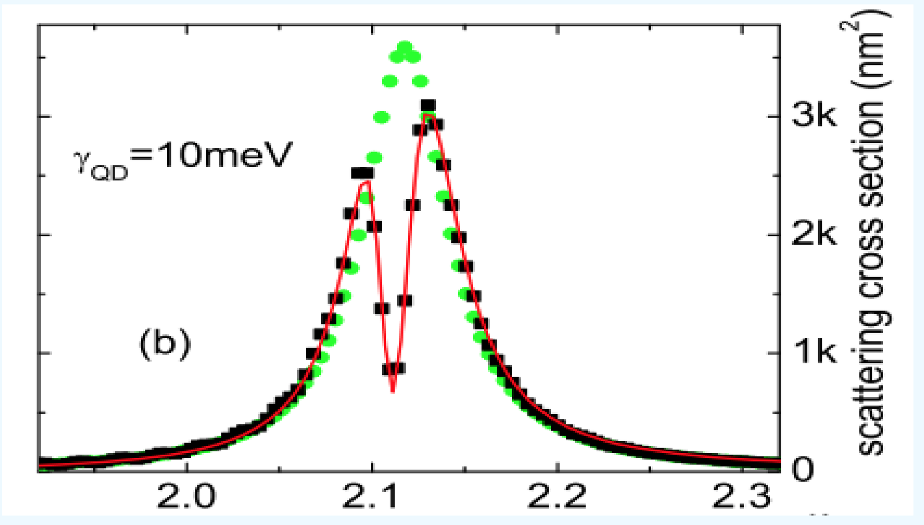
Abstract

The goal of this project is to perform rigorous electromagnetic simulations of two gold nanoparticles coupled to a quantum dot. It has been shown before that coupling two silver nanoparticles to a quantum dot produces a different scattering and absorption spectrum that a single silver nanoparticle exhibits. We are interested in seeing how light will respond to an identical system, but with gold nanoparticles instead of silver. A graduate student working in the same lab will attempt to experimentally measure the scattering and absorption of light on the exact system that I intend to model, whereby after we will be able to compare the calculations I performed to the experimental results. To accurately model this system, a solid quantitative understanding of the coupled electric and magnetic fields inside the gold particle is necessary. To achieve this, I will use a numerical approach such as the Finite-Difference Time-Domain method. This numerical method calculates the electric and magnetic fields by solving Maxwell's Equations directly, making it a very intuitive and flexible method for determining the fields of interest. Once we know the fields, we can then relate these fields to the energy flux over the surface of the metal nanoparticle to yield a clear picture of the absorption and scattering due to the metal nanoparticle. To ensure that our simulations are giving us accurate results, we will first model a single uncoupled silver nanoparticle, as the absorption and scattering spectrum of this system is analytically solvable, letting us tell quantitatively whether our calculations are correct. From there, we will model the two silver nanoparticles coupled to a quantum dot and compare these with previously published results. Once we are confident our simulations are giving us accurate results, we will transition into modeling the desired gold nanoparticle quantum dot system.

Introduction

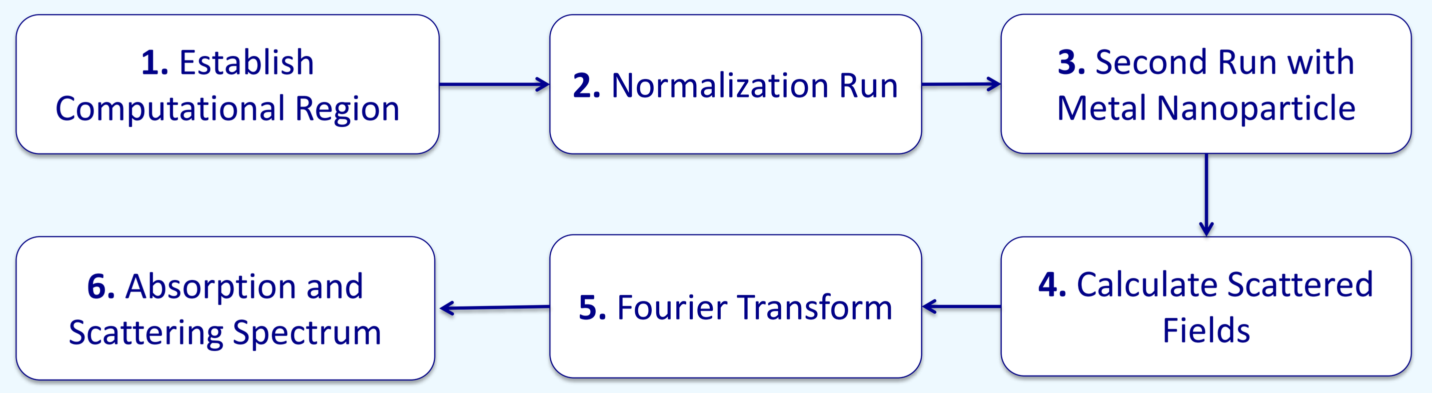
- Plasmons represent the collective electron oscillation inside the plasmonic metal; the frequency of these oscillations is highly dependent on the shape and composition of the metal.
- Plasmons can exhibit strong electromagnetic coupling to light if they are driven by a light pulse at their resonant frequency. Placing two of these metals together in an assembly can lead to strong electromagnetic coupling between the two nanoparticles.
- It has been shown before[1] that you can couple these plasma oscillations to semiconducting nanoparticles (quantum dots) to change how much light is scattered or absorbed by the plasmonic metal.
- We want to analyze the same system but with gold nanoparticles instead of silver and compare and contrast our results.



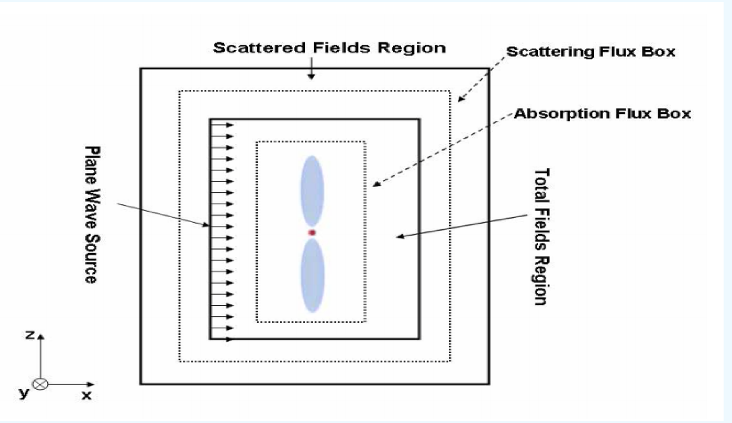
Scattering spectrum of a single silver nanoparticle (green) superimposed on the scattering spectrum of the silver nanoparticle-quantum dot system[1].

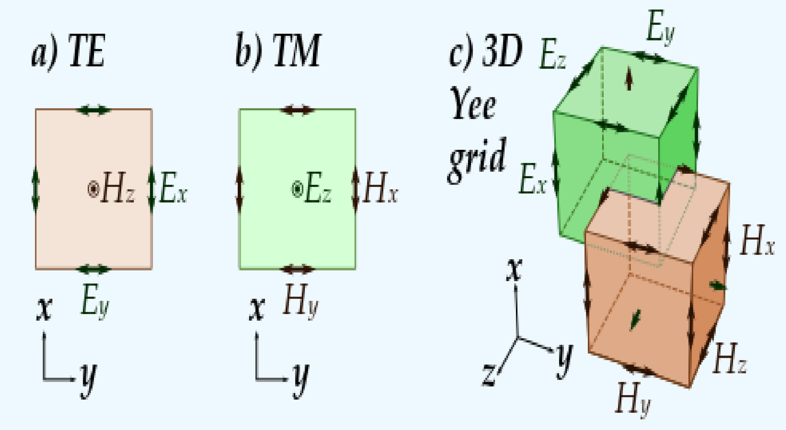
Computational Design & Methods

Finite-Difference Time Domain (FDTD)



- Computational method that numerically calculates the electric and magnetic fields by solving Maxwell's Equations in the time domain.
- Some programs that utilize FDTD are MEEP, Lumerical, and Rsoft. The data generated for this project was all done using MEEP.
- Modeling metals in MEEP requires implementing the dielectric function of a given metal based off the Lorentz-Drude model of metals. This involves six different parameters (two for the Drude model, four for the Lorentz model).

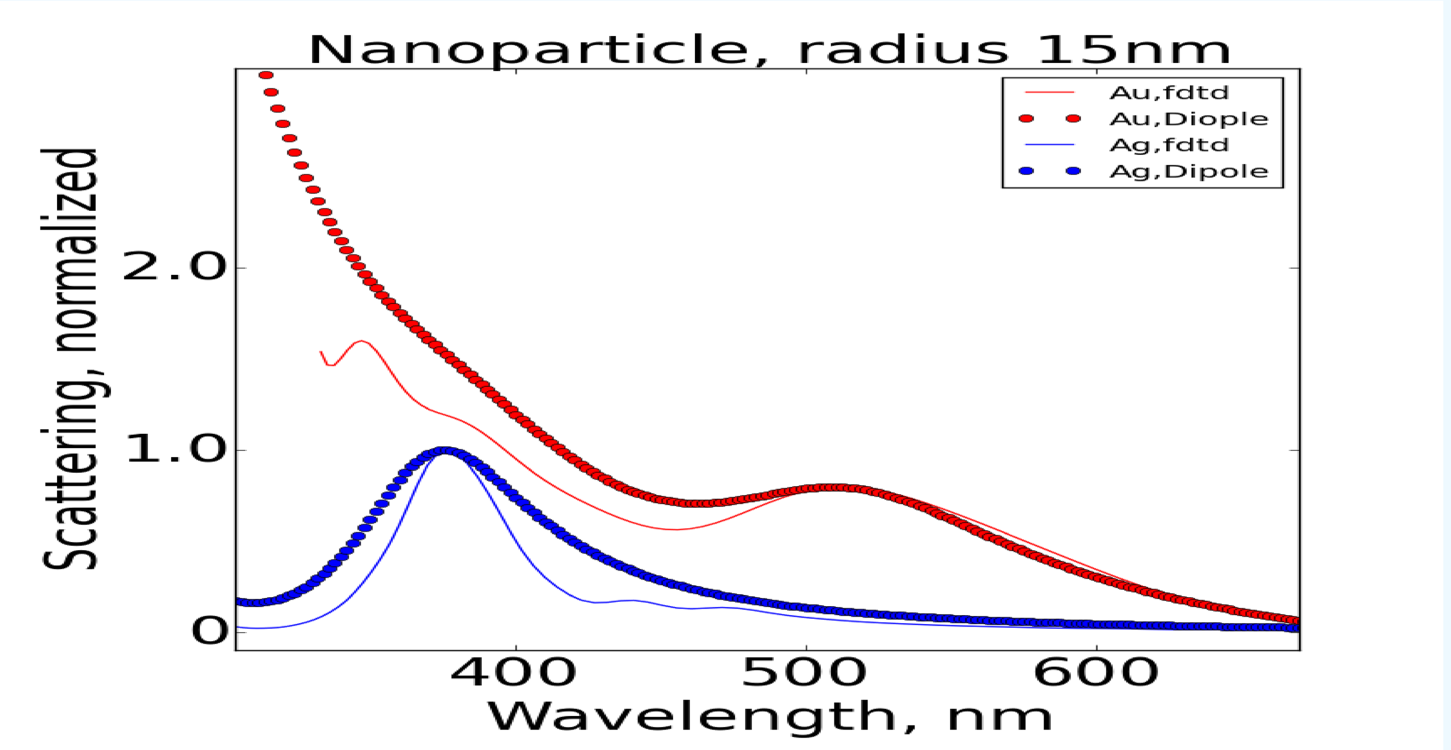




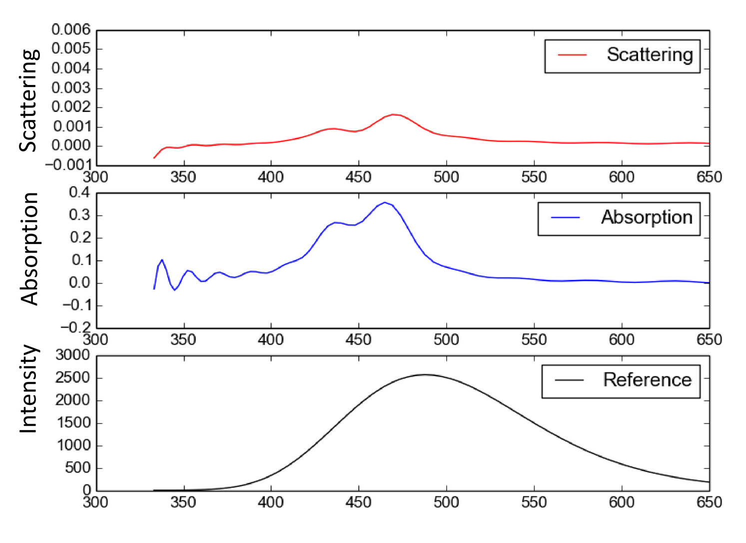
(LEFT[1]) Image of an FDTD computational domain. (RIGHT – Image Credit: Wikipedia) Image off Yee Cells which are the spatial cells used in FDTD to calculate the electric and magnetic fields.

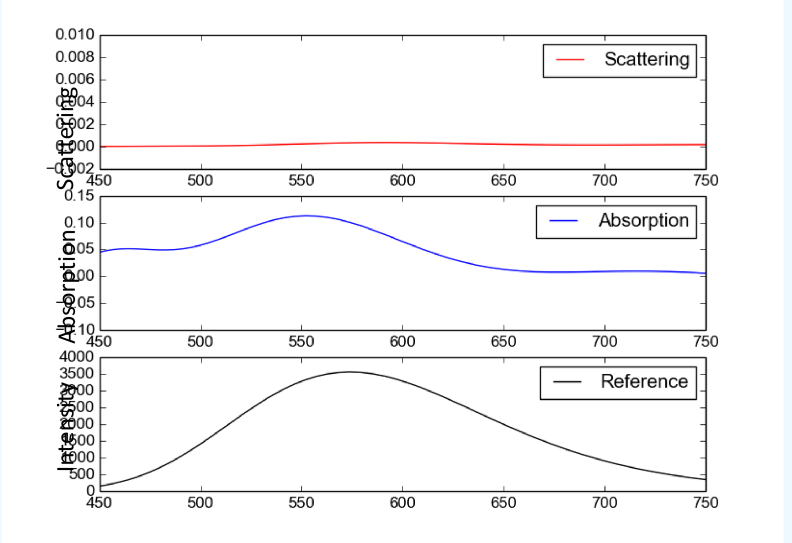
Results

- **Comparison of computational results to analytical results for a silver and gold sphere.**
- **Resonance peak agrees with analytical results for both gold and silver; linewidth for silver peak is different compared to analytical result**

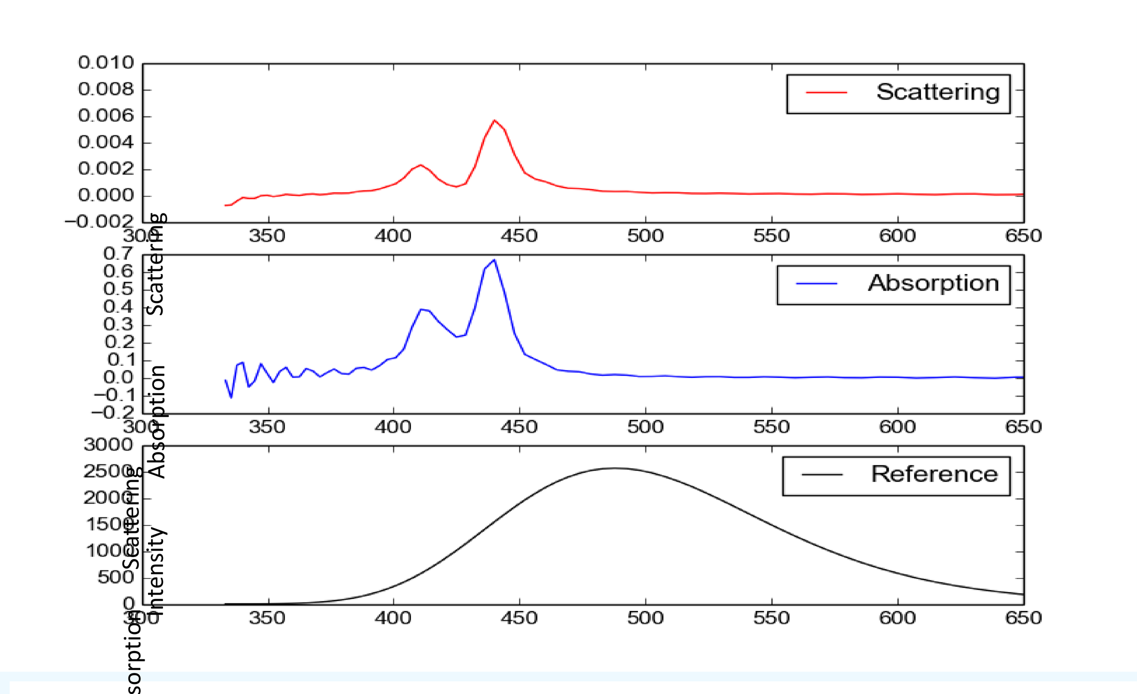


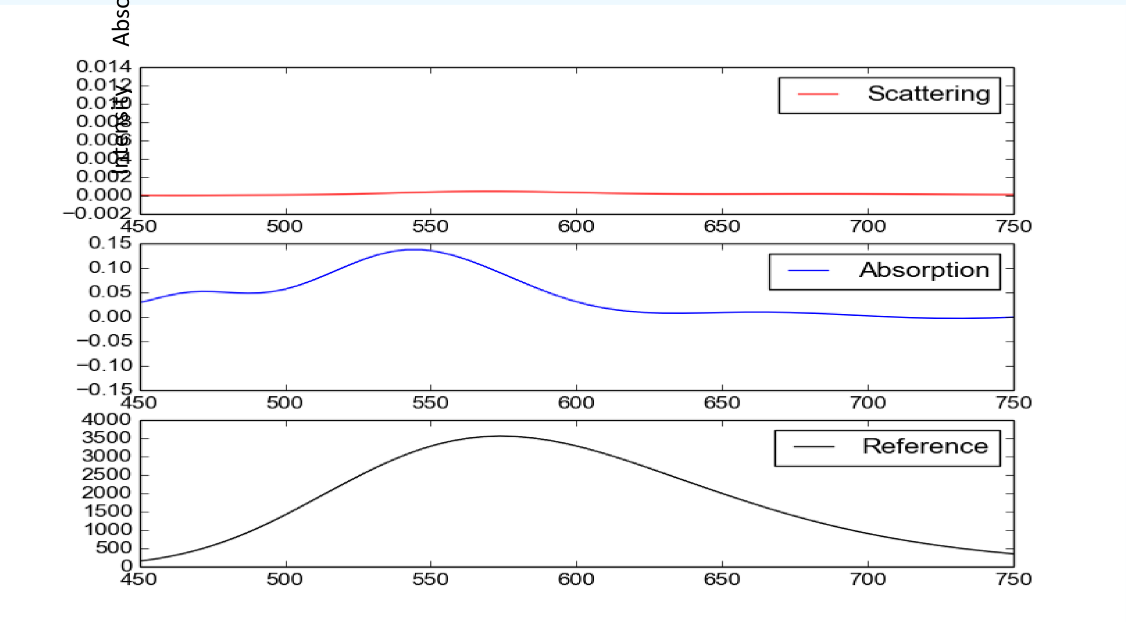
- **Computational results for a silver (LEFT) and gold (RIGHT) ellipsoid using the Lorentz-Drude parameters from[2].**
- **Gold and silver ellipsoids represent the nanoparticles we are trying to model in the assembly. Preliminary results, need to compare to analytical expression.**





- **Computational results for silver (TOP) and gold (BOTTOM) ellipsoid using Lorentz-Drude parameters obtained from fitting the data in[3].**
- **Similar resonances when compared to the previous results, however these simulations results in sharper peaks.**
- **Like before, need to compare to analytical results**





Conclusions & Future Directions

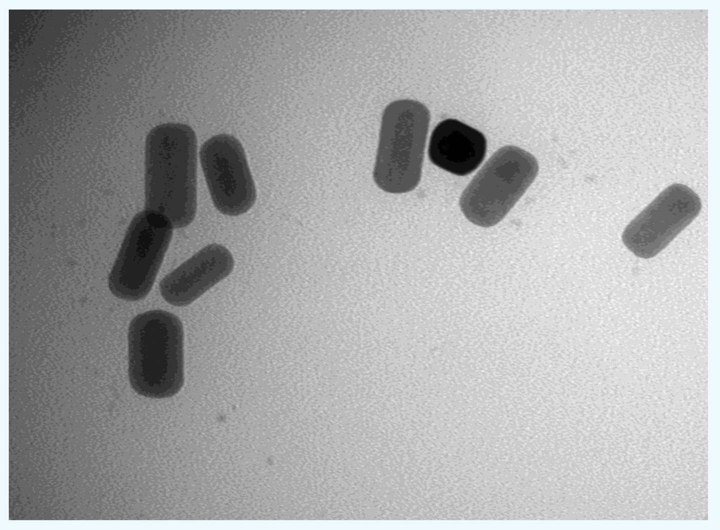
Conclusions

- Currently have a working FDTD code that can generate accurate scattering and absorption spectra
- Have scattering and absorption spectra for ellipsoid shaped nanoparticles

Future Direction

- Incorporate quantum dots into the code and simulate gold and silver nanoparticle assemblies.
- Compare the results of silver to the results obtained in (author, year).
- Compare results of gold to experimental results obtained from a graduate student who intends on doing experimental analysis on the nanoparticle assembly system.

STEM image of gold nanorods and quantum dots used in the experimental analysis of the nanoparticle assembly system.



References:

1. Wu, X.; Gray, S. K.; Pelton, M. Quantum-Dot-Induced Transparency in a Nanoscale Plasmonic Resonator. *Opt. Express* **2010**, *18*, 23633.
2. Rakic, A.; Djurisic, A.; Elazar, J.; Majewski, M. Optical Properties of Metallic Films for Vertical Cavity Optoelectronic Devices. *Applied Optics* **1998**, *37*, 5271-5283
3. Lance, K.; Coronado, E.; Zhao, L.; Schatz, G. The Optical Properties of Metal Nanoparticles: The Influence of Size, Shape, and Dielectric Enviornment. *The Journal of Physical Chemistry* **2003**, *107*, 668-677