Introduction

- Classical electrodynamic code for solving Maxwell’s Equations to obtain the electric field and the magnetic field, e.g.,
  \[ \nabla \times H = \frac{\partial D}{\partial t} \\
\nabla \times E = -\mu_0 \frac{\partial H}{\partial t} \]

- Noble metal “nanoantennas”: near-field light intensity enhanced ~1000 X
- Useful in: cancer therapy, solar cells, meta-materials, chemical sensing, etc
- Large size of nanoparticles, (~ millions atoms) preclude quantum description and allows for classical modeling via Maxwell’s Equations
- Initial question: How does particle size dictate absorption?

Simulation Box

- Box that simulates vacuum space on the inside.
- Boundary: absorbs the light radiated when the metal nanoparticle is excited with light.

Results

- Motion of the electric field following the pulse as it moves forward in time.

- Total current in the nanoparticle following excitation

- As the grid spacing becomes smaller the answer converges.

- Decreased absorption with decreasing nanoparticle size

- As the size of the nanoparticle increases it absorbs different Frequencies.
- A smaller nanoparticle emits a red color and as it increases in size it appears blue.

Program Flow

- We solve this equations on a grid using finite differences for the spatial derivatives.
- For this code we used Open MP to parallelize the code.
- We are solving for Maxwell’s Equations in the 3D so we can parallelize over the finite differences.

References

- Thank you to Dr. Kenneth Lopata and Holden Smith for their guidance during this REU.
- This material is based upon work supported by the National Science Foundation under award OCI-1263236 with additional support from the Center for Computation & Technology at Louisiana State University.