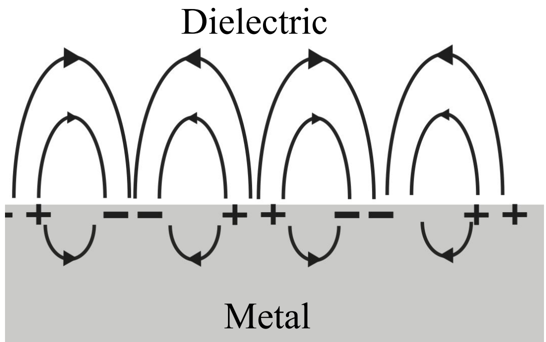
Scattering by Penetrable Spheres with NGSolve

Benjamin J. Latham

CLOVERS
Carvalho Lab for exOtic waVes in Electromagnetics, Resonances and Scattering

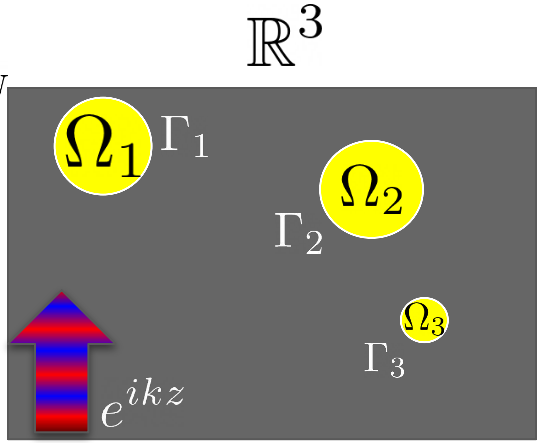
Motivation

1. Our goal is to numerically observe surface plasmons
   a. Highly oscillatory, localized to the interface electromagnetic waves
   b. Very difficult to capture with lab experiments due to extreme localization/oscillations
   c. Numerical models may be very useful to inform experiment
2. In particular, we will be focusing on **spheres** suspended in a dielectric
   a. For example, gold nanoparticles in vacuum
   b. Problems like this can occur physically, for example when using Raman Spectroscopy to image molecules
   c. In order to examine these, we need to first solve the scattering problem in this setting.



The Problem

Suppose we have N spheres suspended in $\mathbb{R}^3$, labeled as $\Omega_1, \Omega_2, ...\Omega_N$
with as many respective borders $\Gamma_1, \Gamma_2, ...\Gamma_N$



We seek to solve a modified Helmholtz equation:

$$\nabla \cdot (\epsilon^{-1} \nabla u) + k^2 u = 0, u \in H^1_{loc}(\mathbb{R}^3)$$

Where the solution is the sum of an incident plane wave and the resulting scattered wave.

$$u = u^{inc} + u^{sca} \qquad u^{inc} = e^{ikz}$$

We also demand a transmission condition over the interface between the spheres and the dielectric:

$$[u]_{\Gamma_k} = [\epsilon^{-1} \partial_n u]_{\Gamma_k} = 0 \text{ for } k \in 0, 1, 2...N$$

Lastly, we need a boundary condition at infinity for our scattered field, here we use the Sommerfeld radiation condition for waves:

$$\lim_{r \to \infty} r(\partial_r - ik) u^{sca} = 0$$

Absorbing Boundary Condition

We would like to treat this problem numerically with the Finite Element Method (FEM). Consequently, we must artificially truncate the domain from $\mathbb{R}^3$.

Let our truncated domain be given by $\mathbb{D} = B_R(O)$ (Ball of radius R at the origin)

with $\Omega_1, \Omega_2, ..., \Omega_N \subset \mathbb{D}$.

In order to model the radiation condition in our boundary, for the experiments presented today, I use the first order Feng absorbing boundary condition, given below.[1]

$$\partial_n u^{sca} - (ik - \frac{1}{R})u^{sca}\Big|_{\partial D} = 0$$

[1]: J. J. Shirron, I. Babuška, A comparison of approximate boundary conditions and infinite element methods for exterior Helmholtz problems. Computer Methods in Applied Mechanics and Engineering, Volume 164, Issues 1–2, 1998

Weak Formulation

As part of setting up FEM, we now seek a weak formulation to the below problem

$$u \in H^1(\mathbb{D})$$

$$\nabla \cdot (\epsilon^{-1} \nabla u) + k^2 u = 0$$

Let v be an arbitrary test function in $H^1(\mathbb{D})$

Taking the expected step of multiplying by v and integrating over the domain gives:

$$-\int_{\mathbb{D}} \epsilon^{-1} \nabla v \nabla u \; d\mathbb{D} + \int_{\partial\mathbb{D}} \epsilon^{-1} v \partial_n u \; dS + \int_{\mathbb{D}} k^2 v u \; d\mathbb{D} = 0$$

Weak Formulation

$$-\int_{\mathbb{D}} \epsilon^{-1} \nabla v \nabla u \; d\mathbb{D} + \int_{\partial\mathbb{D}} \epsilon^{-1} v \boxed{\partial_n u} \; dS + \int_{\mathbb{D}} k^2 v u \; d\mathbb{D} = 0$$

Recall from earlier:

$$\partial_n u^{sca} - (ik - \frac{1}{R}) u^{sca} \Big|_{\partial\mathbb{D}} = 0$$

$$u = u^{inc} + u^{sca}$$

Combining these two gives $$\partial_n u^{sca} = iku - \frac{1}{R} u + \frac{1}{R} u^{inc} - iku^{inc} \Big|_{\partial\mathbb{D}}$$

$$-\int_{\mathbb{D}} \epsilon^{-1} \nabla v \nabla u \; d\mathbb{D} + \int_{\partial\mathbb{D}} \epsilon^{-1} v (iku - \frac{1}{R} u) \; dS + \int_{\mathbb{D}} k^2 v u \; d\mathbb{D} = \int_{\partial\mathbb{D}} \epsilon^{-1} v (-\partial_n u^{inc} - \frac{1}{R} u^{inc} + iku^{inc}) \; dS$$

Weak Formulation

The associated weak formulation problem can then be written:

Find $u \in H^1(\mathbb{D})$ such that $a(u,v) = l(v)$ for v an arbitrary function in $H^1(\mathbb{D})$

$$l(v) = \int_{\partial\mathbb{D}} \epsilon^{-1} v(-\partial_n u^{inc} - \frac{1}{R}u^{inc} + iku^{inc})\ dS$$

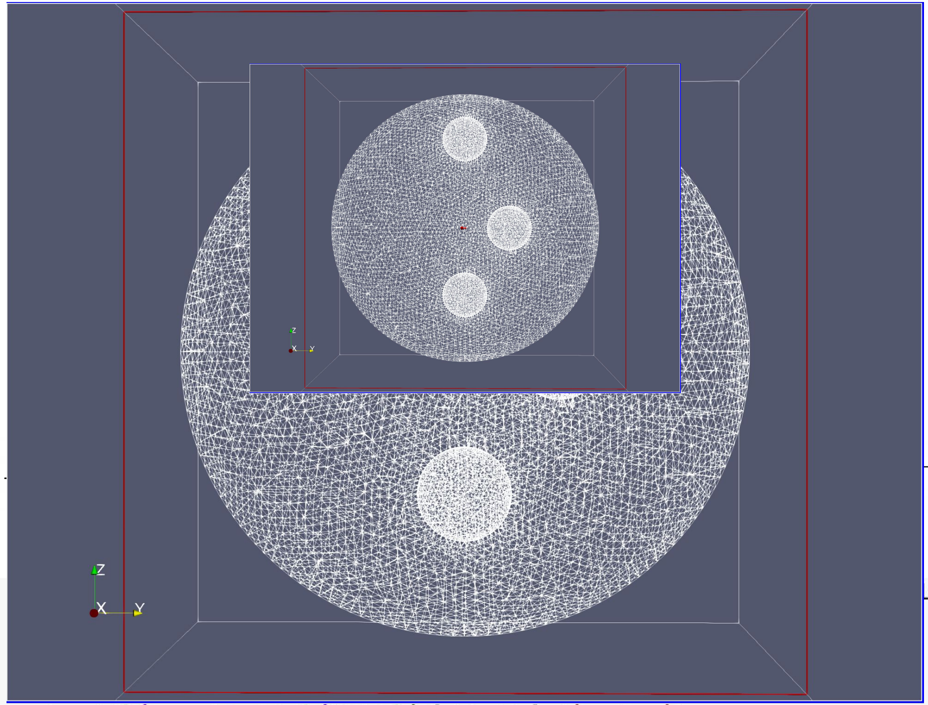
$$a(u,v) = -\int_{\mathbb{D}} \epsilon^{-1} \nabla v \nabla u\ d\mathbb{D} + \int_{\partial\mathbb{D}} \epsilon^{-1} v(iku - \frac{1}{R}u)\ dS + \int_{\mathbb{D}} k^2 vu\ d\mathbb{D}$$

This problem is well-posed for the vast majority of parameters.[2] It can be furthermore shown using Céa's lemma that the FEM has convergent error.

[2]: Bonnet-Ben Dhia, A.-S., Chesnel, L., Ciarlet, P. (2012). T-coercivity for scalar interface problems between dielectrics and metamaterials

Implementation with NGSolve

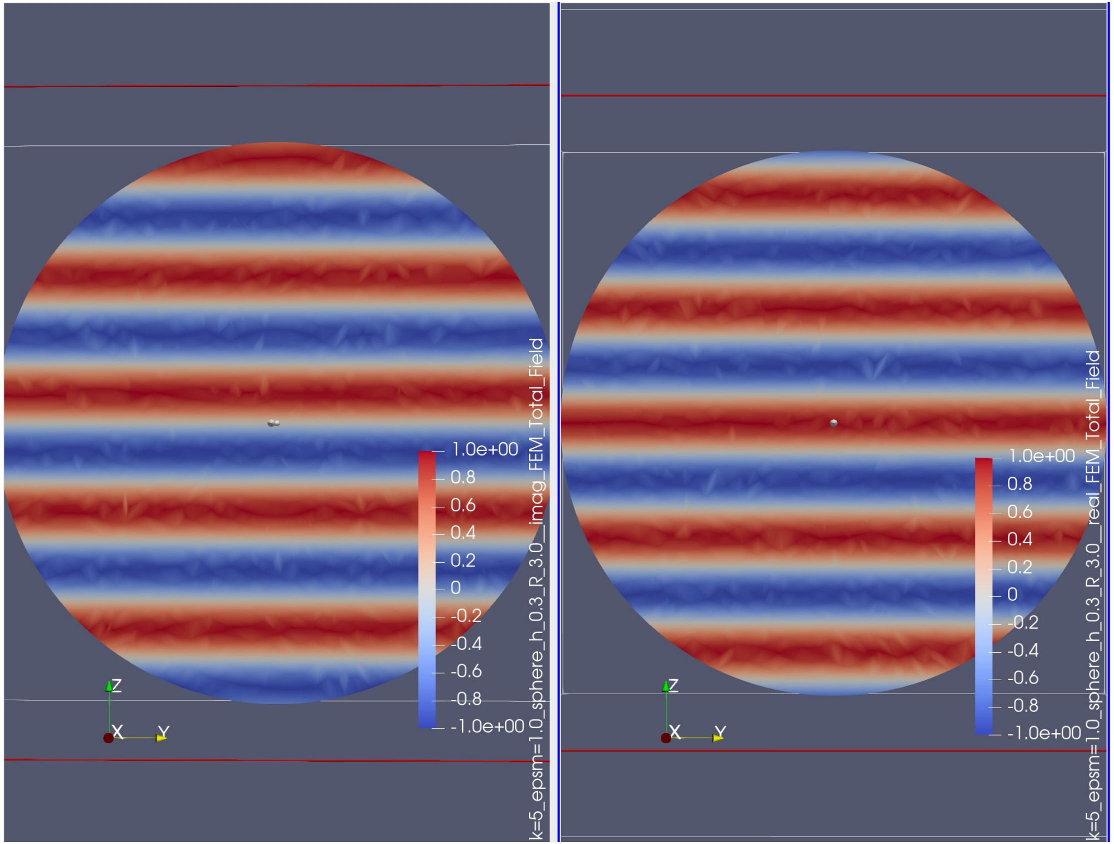
In order to construct a mesh, we make use of the GMSH software, which can build unstructured meshes from a given geometry.

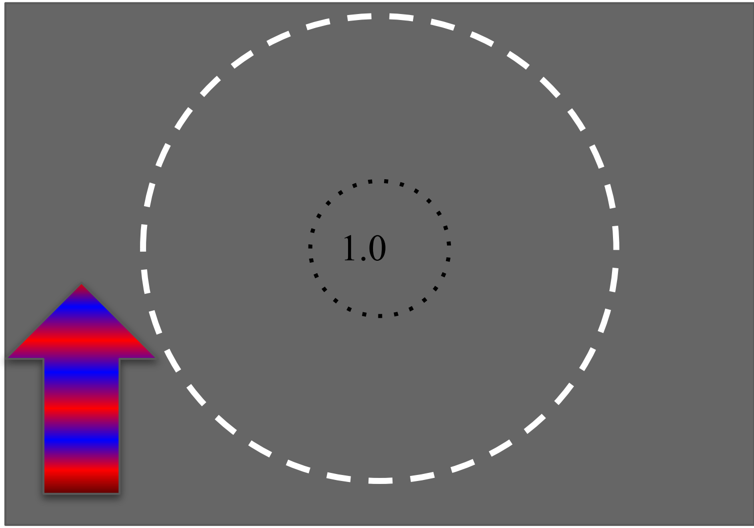


$$l(v) = \int_{\partial \mathbb{D}} \epsilon^{-1} v(-\partial_n u^{inc} \quad \cdots \quad {}^{-1} v(iku - \frac{1}{R}u)\; dS + \int_{\mathbb{D}} k^2 vu \; d\mathbb{D}$$

```
.f.Inc)
a += ((1/epsv)*u*(-1/(R)+1j*k)*v)*ds('outer')
```

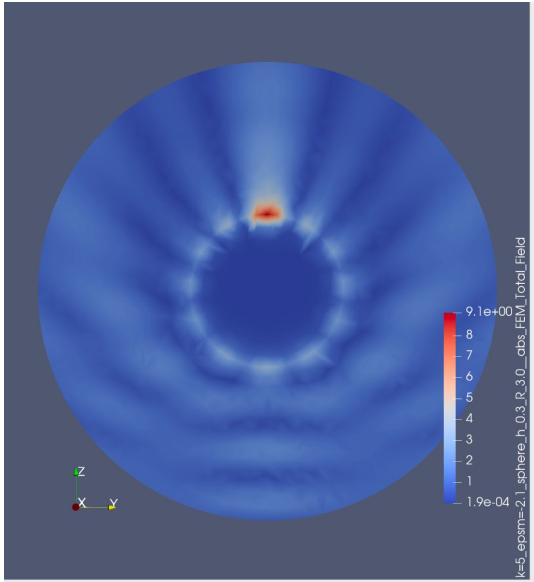
Verification with fictional sphere

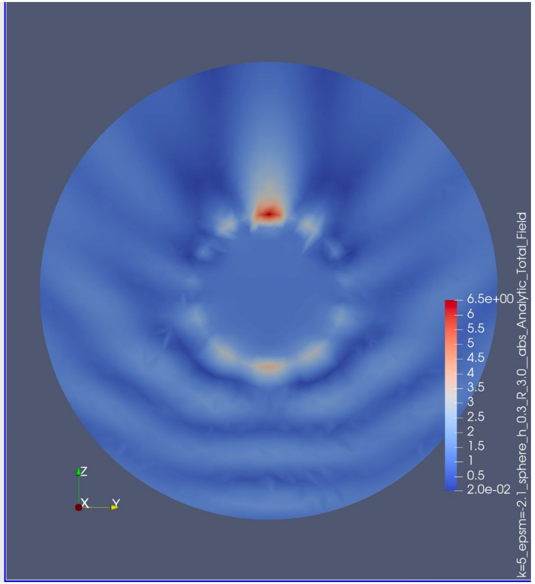


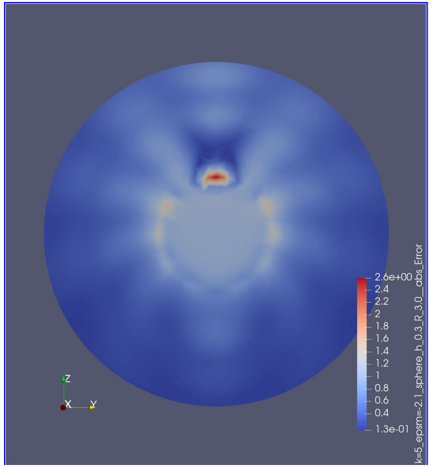


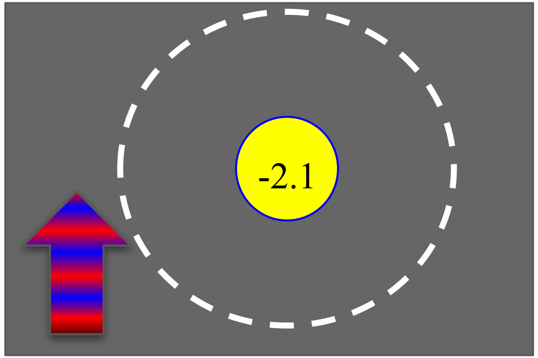
- Order of Finite Element = 4
- # of DOF = 254390
- k = 5
- L2 norm of error = 10^{-3}

Experiment with one sphere

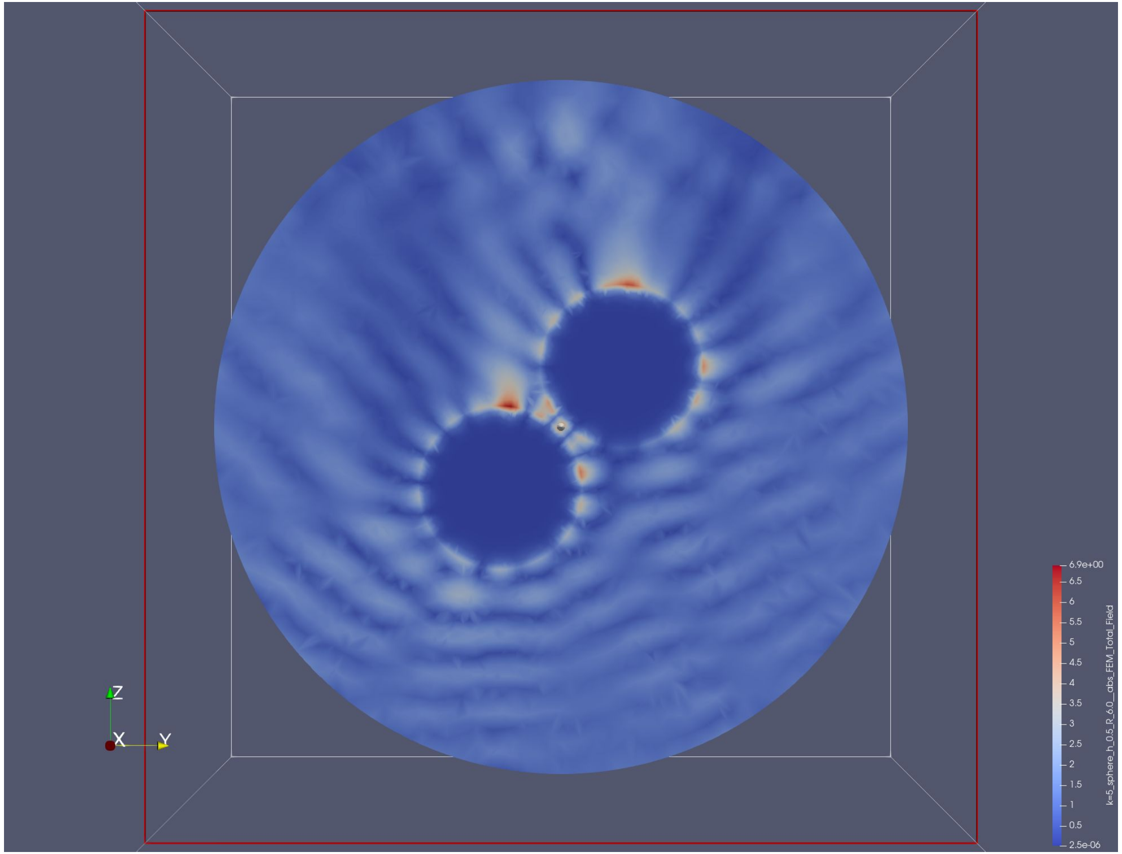


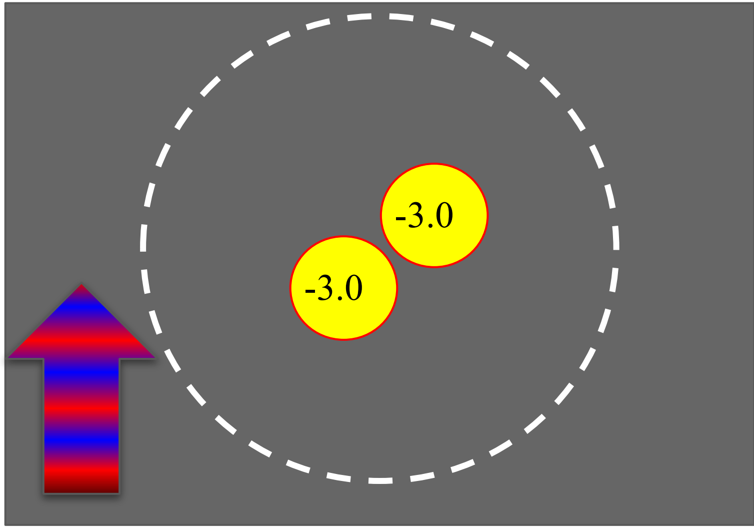




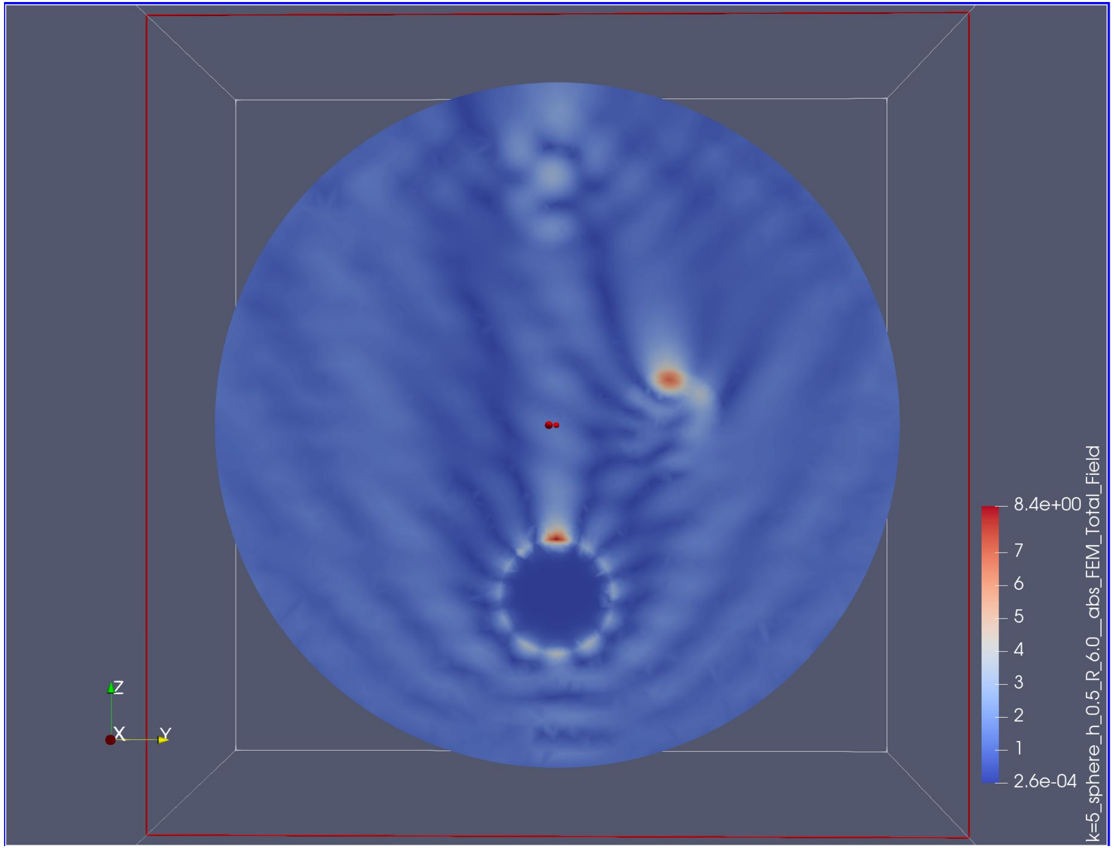


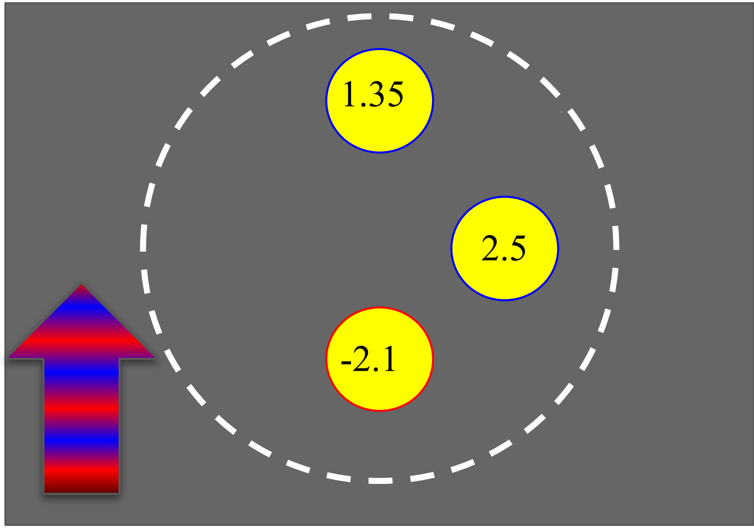
- Order of Finite Element = 3
- # of DOF = 286211
- k = 5





- Order of Finite Element = 2
- # of DOF = 254390
- k = 5





- Order of Finite Element = 2
- # of DOF= 222609
- k= 5

Remaining work to do

- Current results look promising, but the code is still a work in progress, need to investigate better boundary conditions
- There is also the matter of the Plasmon - here, we show various scattering problems, but in order to generate the surface plasmon, there exists a relationship between our choice of k and epsm. Work needs to be done to establish this relationship and test how the code handles the extreme behavior of the surface plasmon.
- For context in the 2d planar case, see my previous seminar - https://appliedmath.ucmerced.edu/seminars/imaging-and-sensing/waves

New Directions for this code

- Some interest in using boundary integral methods to capture accurately the infinite behavior outside of the solution
- Lastly, when spheres are closely situated the interfering waves can be very difficult to model numerically without extremely refined meshes, so there is interest in handling the plasmonic behavior analytically and subtracting it out, then solving for the remaining portion of the solution, which is hopefully easier to compute numerically.