Modeling Plasmons

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1 Introduction

This brief overview details solving wave-equations,specifically the Plasmon Wave Equation, with a Finite Element Method through the Python package FEniCS. The final result is a intuitive API for simulating Plasmons along with an interactive Bokeh Application for simulating Plasmons to allow experimental measurements to be compared to these theoretical predictions.

2 Time Independent Schrödinger Equation

$$\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x},t) + V(\vec{x})\psi(\vec{x},t) = i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t} \tag{1}$$

For the time independent Schrödinger equation this transforms into

$$\frac{\hbar^2}{2m}\nabla^2\psi(\vec{x}) + V(\vec{x})\psi(\vec{x}) = E\psi(\vec{x}) \tag{2}$$

This is an eigenvalue equation where the left hand side is a Hamiltonian operator acting on the wave functions $\psi_n(x)$ and eigenvalues E_n.

For the harmonic oscillator problem we have

$$U(\vec{x}) = \frac{1}{2}k\vec{x}^2$$

Through some additional simplifications (specifically scaling the x term) we can achieve the following equation.

$$\nabla^2\psi(\vec{x}) + (\epsilon - \vec{x}^2)\psi(\vec{x}) = 0 \tag{3}$$

In order to translate this into Fenics to be solved as an eigenvalue problem, we need to obtain the weak variational form. Going forward we will be solving this problem in 1-D.

2.0.1 1-D Solution

$$\frac{\partial^2}{u}\partial x^2 + (k - x^2)u = 0$$

$$\int_\Omega \frac{\partial^2}{u}\partial x^2 + (k - x^2)udx = 0$$

With integration by parts, we can show that;

$$\int_\Omega \frac{\partial^2 u}{\partial x^2} vdx = \int_{\partial\Omega} (\frac{\partial u}{\partial x} \cdot n)vds - \int_\Omega \frac{\partial u}{\partial x}\frac{\partial v}{\partial x}dx$$

We have the boundary terms defined to go to zero.

$$\int_{\partial\Omega} \frac{\partial u}{\partial x} vds = 0$$

The result is this following equation.

$$\int_\Omega \frac{\partial^2 u}{\partial x^2} vdx = - \int_\Omega \frac{\partial u}{\partial x}\frac{\partial v}{\partial x}dx$$

Plugging this into our main equation yields:

$$\int_\Omega \frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + x^2 udx = \int_\Omega kuvdx \tag{4}$$

2.1 Helmholtz Equation

The Helmholtz equation is as follows:

$$\nabla^2 u + k^2 u = 0$$

Then casting to weak form to solve the variational problem:

$$\int_\Omega (\nabla^2 u)v + \int_\Omega k^2 uv = 0 \int_\Omega \nabla u \nabla v + \int_\Omega k^2 uv \qquad = 0$$

We can then solve this variational problem with the SLEPcEigensolver since the Helmholtz equation is really eigenvalue/vector problem. These are the theoretical solutions obtained.

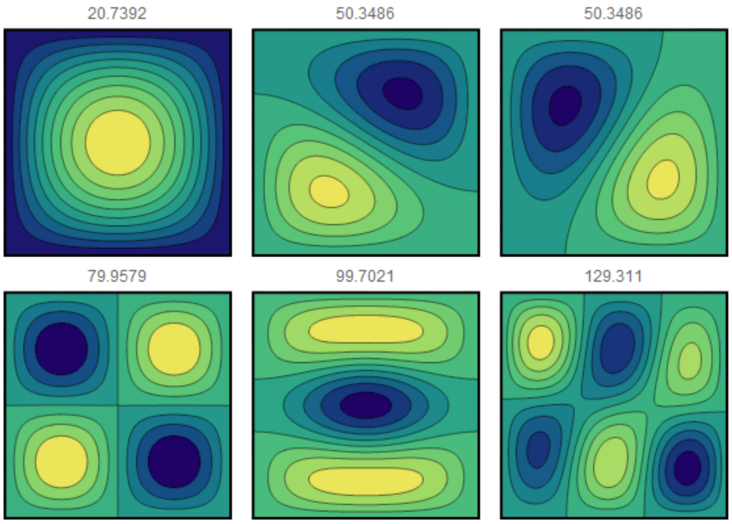


Figure 1: Theoretical solutions to the Helmholtz equations with associated eigenvalues.

And here are the solutions that we extracted:

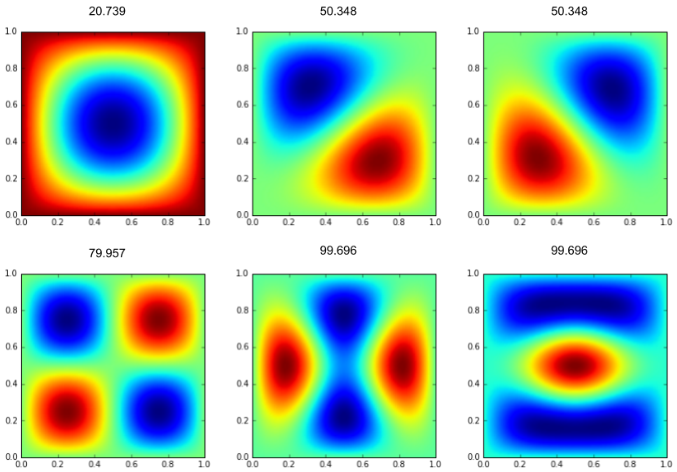


Figure 2: Calculated solutions to the Helmholtz equations with associated eigenvalues. We see there is a slightly different calculated solution for the eigenvalue equal to 99.696.

2.2 Modeling Plasmons

Our plasmon wavefunction looks like one of the following equations [1]:

$$\Phi_{ind}(r,\theta) = \frac{\kappa}{2\pi} V * \nabla \cdot [\frac{1}{q_p(r,\theta)} \nabla \Phi(r,\theta)] \tag{5}$$

$$\Phi_{ext}(r,\theta) = \Phi(r,\theta) + \frac{i\sigma}{\omega} \nabla^2 \Phi(r,\theta) \tag{6}$$

Where we have κ, V as the coulomb kernel, σ, ω, q_p.

In this case we can have complex values for σ and for our solution Φ. Therefore we need to rephrase the problem into a system of coupled differential equations.

If we consider equation 4 from [1] $q_p(r,\theta) = \frac{i\kappa\omega}{2\pi\sigma}$. Since we have $q_p(r,\theta) = \frac{1}{\lambda} + i\frac{1}{L}$. We can calculate σ_1 and σ_2 from $\sigma = \sigma_1 + i\sigma_2$.

$$\sigma_1 = \frac{\frac{1}{L}}{(\frac{1}{\lambda^2} + \frac{1}{L^2})},\ \sigma_2 = \frac{\frac{1}{\lambda}}{(\frac{1}{\lambda^2} + \frac{1}{L^2})},\ \omega = \frac{2\pi}{\kappa V}$$

These establish the relationship between the physical values and the the coefficients σ_1, σ_2, and ω.

Now with $\sigma = \sigma_1 + i\sigma_2$ and $\Phi = u_1 + iu_2$ we can plug into equation (6) with $\Phi_{ext}(r,\theta) = 0$.

$$\omega(u_1 + iu_2) = (i\sigma_1 - \sigma_2)\nabla^2(u_1 + iu_2) \tag{7}$$

Through a couple of simple algebraic manipulations we get the following coupled differential equations.

$$(\sigma_1^2 + \sigma_2^2)\nabla^2 u_1 = \omega(\sigma_1 u_2 - \sigma_2 u_1) \tag{8}$$

$$(\sigma_1^2 + \sigma_2^2)\nabla^2 u_2 = -\omega(\sigma_1 u_1 + \sigma_2 u_2) \tag{9}$$

Now we can phrase the two coupled equations in weak form.

$$\int_\Omega (\sigma_1^2 + \sigma_2^2)\nabla u_1 \cdot \nabla q \, dx + \omega \int_\Omega (\sigma_1 u_2 - \sigma_2 u_1) q \, dx = 0 \quad \forall q \in V \tag{10}$$

$$\int_\Omega (\sigma_1^2 + \sigma_2^2)\nabla u_2 \cdot \nabla v \, dx - \omega \int_\Omega (\sigma_1 u_1 + \sigma_2 u_2) v \, dx = 0 \quad \forall v \in V \tag{11}$$

3 Simulation Results

We can now specify parameter values for λ and L while keeping $\omega = 2\pi$. We find that larger the value for L, the smaller the overall damping.

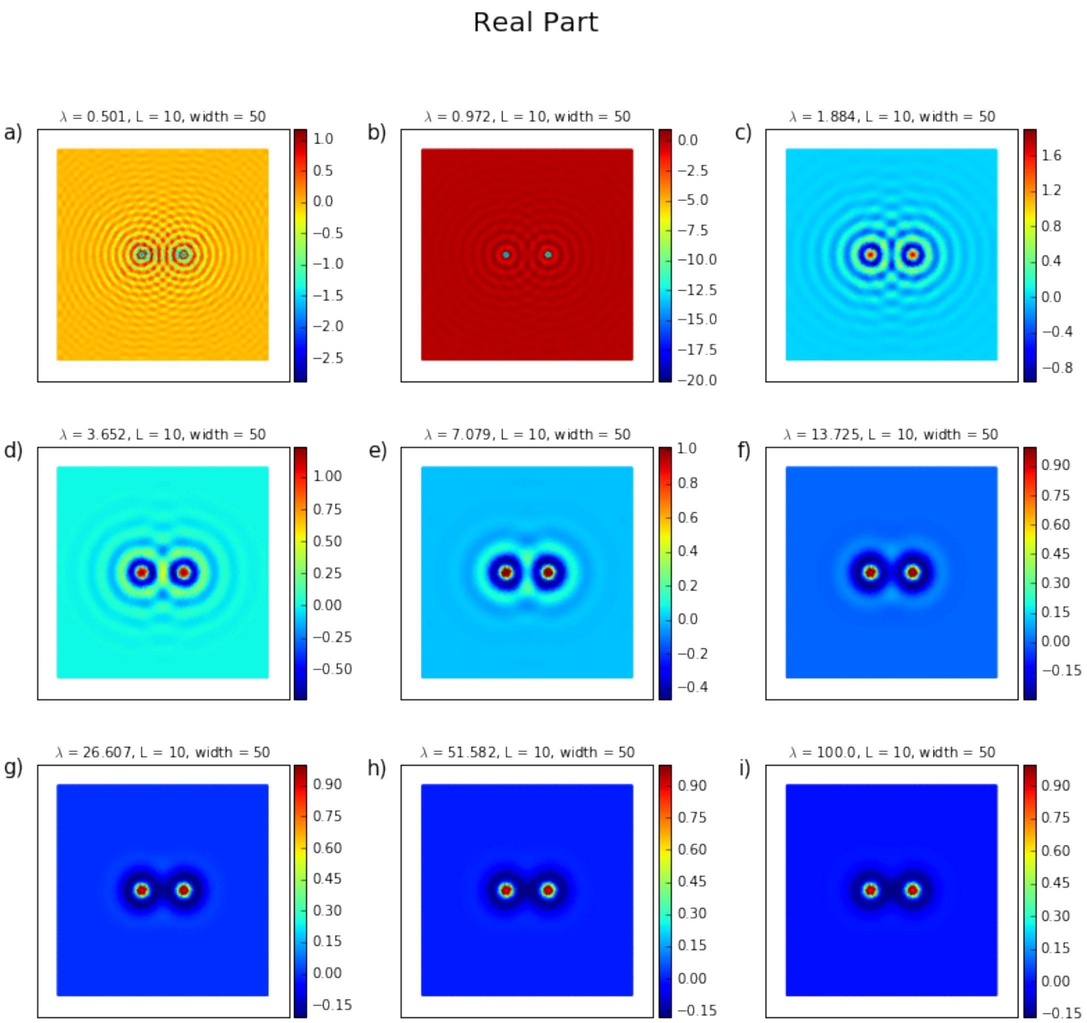
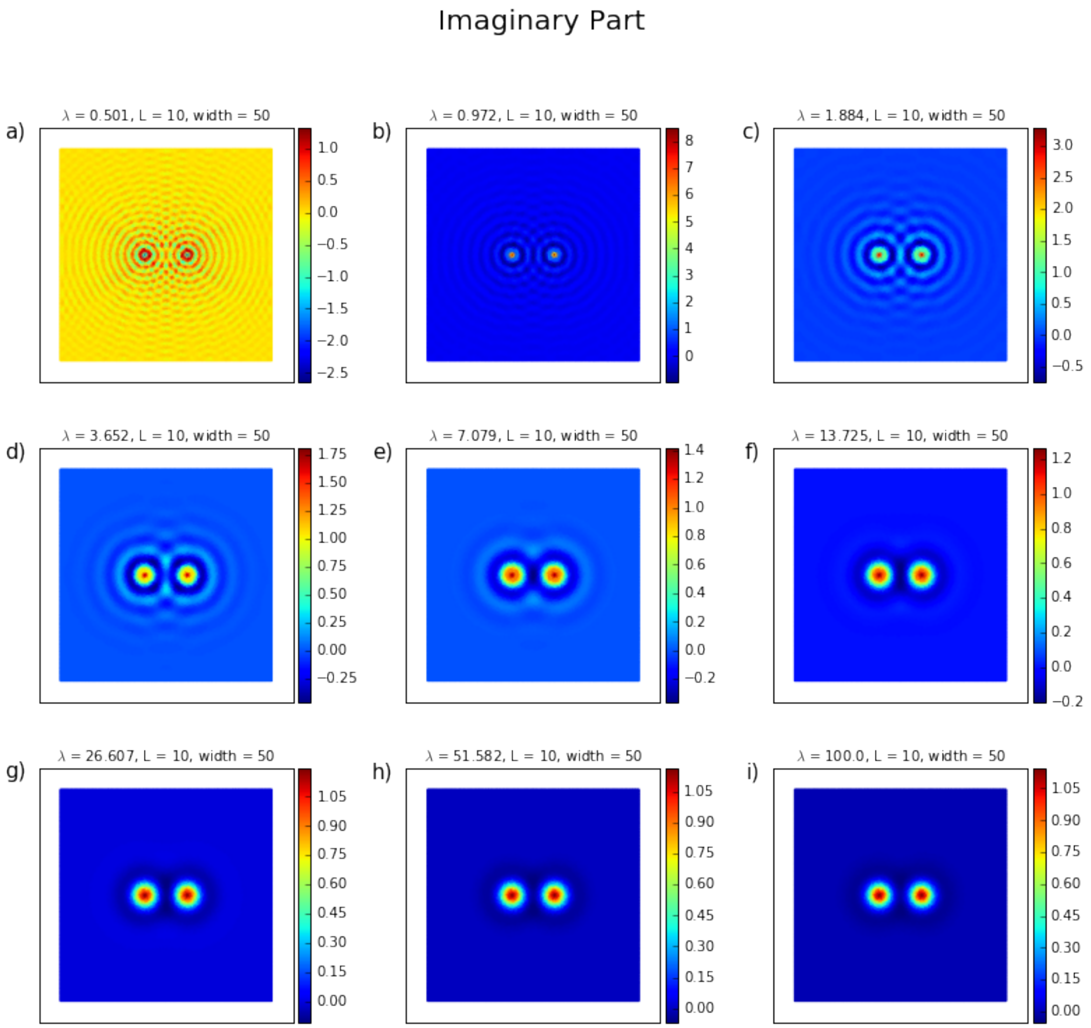


Figure 3: Here L = 10. Real solutions with the specified parameters are plotted. There are two circular sources with Dirichlet boundary conditions in the middle of the sample.


Imaginary Part

a) λ = 0.501, L = 10, width = 50

b) λ = 0.972, L = 10, width = 50

c) λ = 1.884, L = 10, width = 50

d) λ = 3.652, L = 10, width = 50

e) λ = 7.079, L = 10, width = 50

f) λ = 13.725, L = 10, width = 50

g) λ = 26.607, L = 10, width = 50

h) λ = 51.582, L = 10, width = 50

i) λ = 100.0, L = 10, width = 50

Figure 4: Here L = 10. Imaginary solutions with the specified parameters are plotted. There are two circular sources with Dirichlet boundary conditions in the middle of the sample.

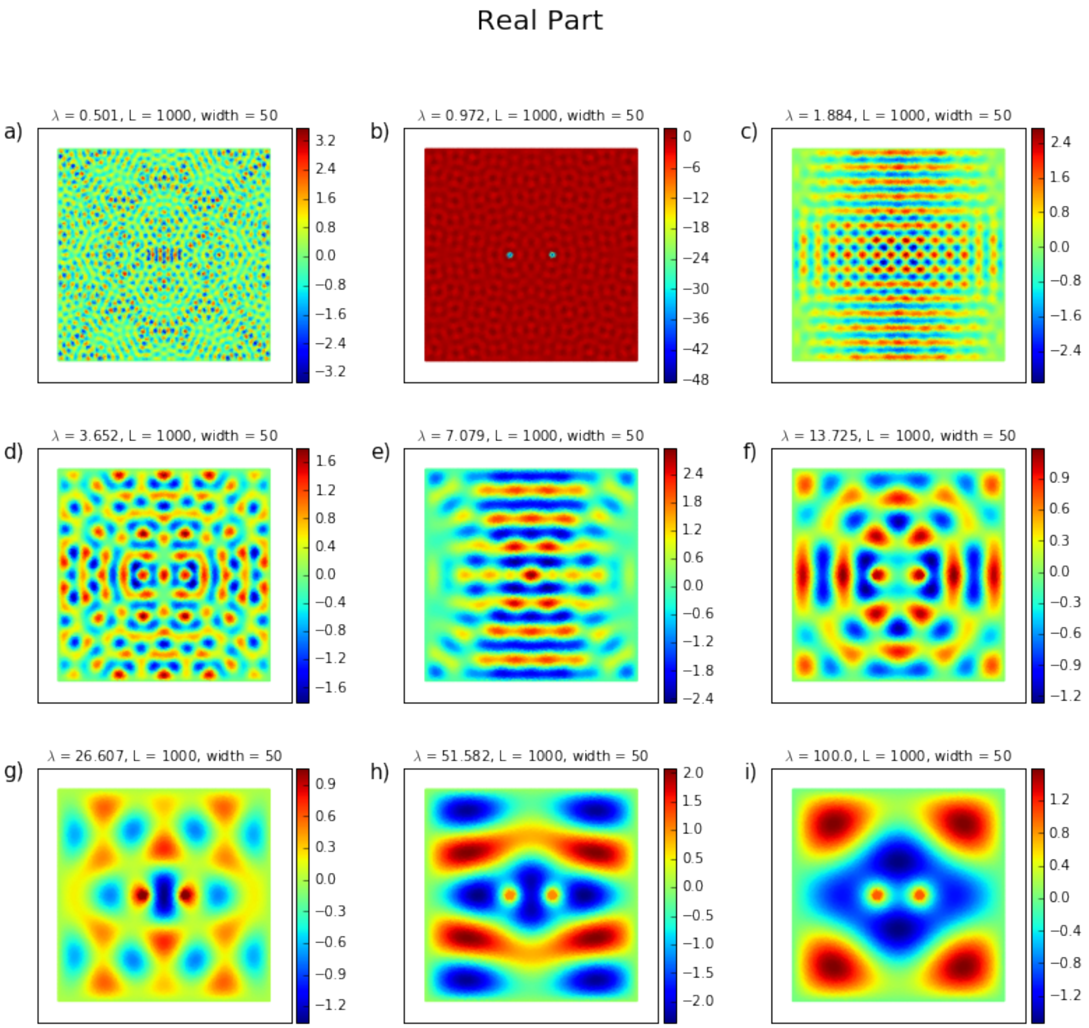


Figure 5: Here L = 1000. Real solutions with the specified parameters are plotted. There are two circular sources with Dirichlet boundary conditions in the middle of the sample.

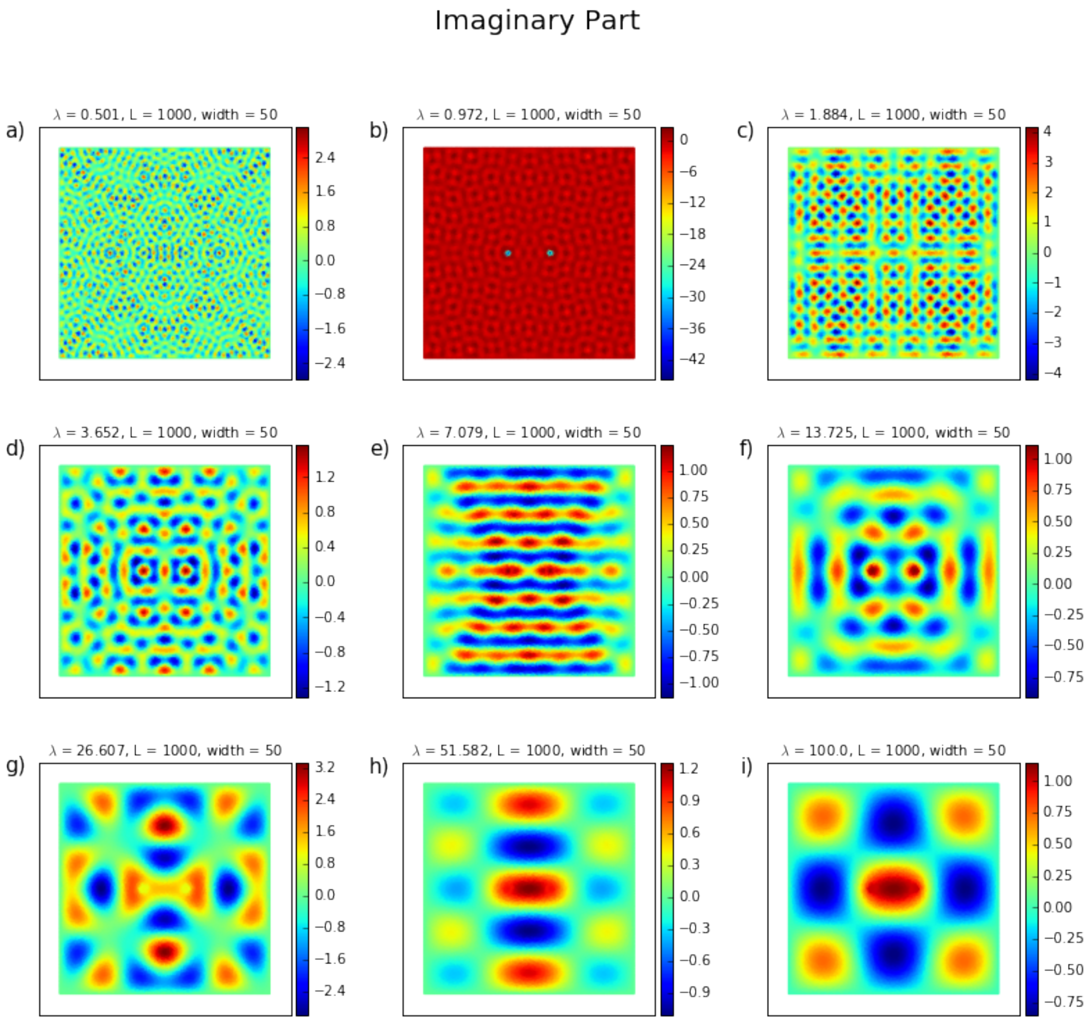


Figure 6: Here L = 1000. Imaginary solutions with the specified parameters are plotted. There are two circular sources with Dirichlet boundary conditions in the middle of the sample.

3.1 Sample Creation Program

So far

```
#Preparing Sample
sample = RectangularSample(50,100)
sample.placeCircularReflector(10,40,5.0)
sample.placeCircularReflector(15,40,5.0)
sample.placeCircularReflector(20,40,5.0)
sample.placeCircularReflector(25,40,5.0)
sample.placeCircularReflector(30,40,5.0)
sample.placeCircularReflector(35,40,5.0)
sample.placeCircularReflector(40,40,5.0)
sample.placeCircularSource(30.0,25,2.0)
sample.placeCircularSource(20.0,25,2.0)


#initializing parameters
sigma = S()
omega = O()

#arg0 = \lambda, arg1 = L
sigma.set_sigma_values(1,10)
#arg0 = \kappa, arg1 = V
omega.set_omega_values(1,1)

sample.run(omega,sigma,density = 200)
```

With this code, we create an array of reflectors and two circular sources. The mesh and solutions are visualized below:

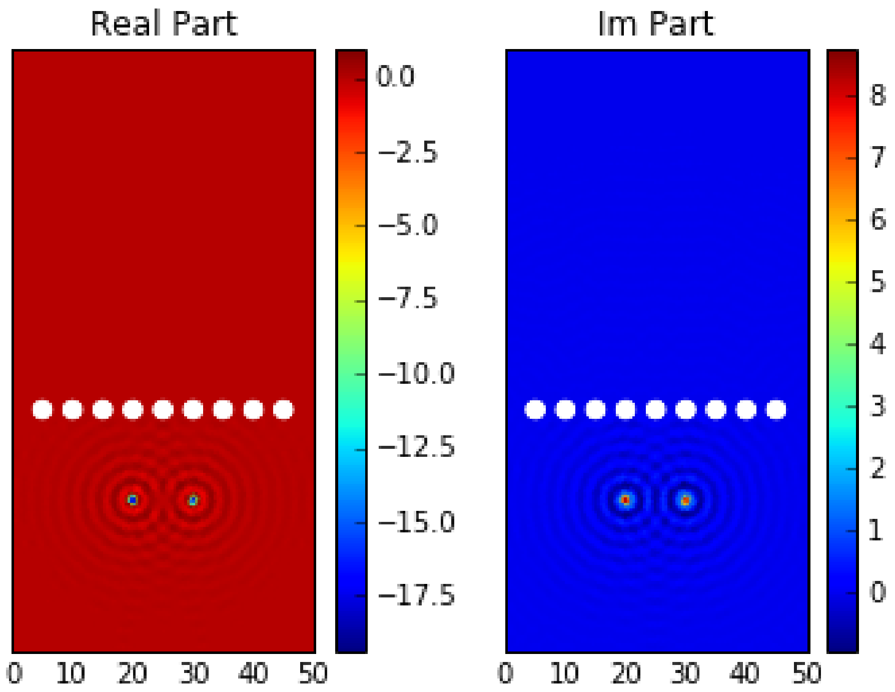


Figure 7: Here $\lambda = 1$, L = 10.

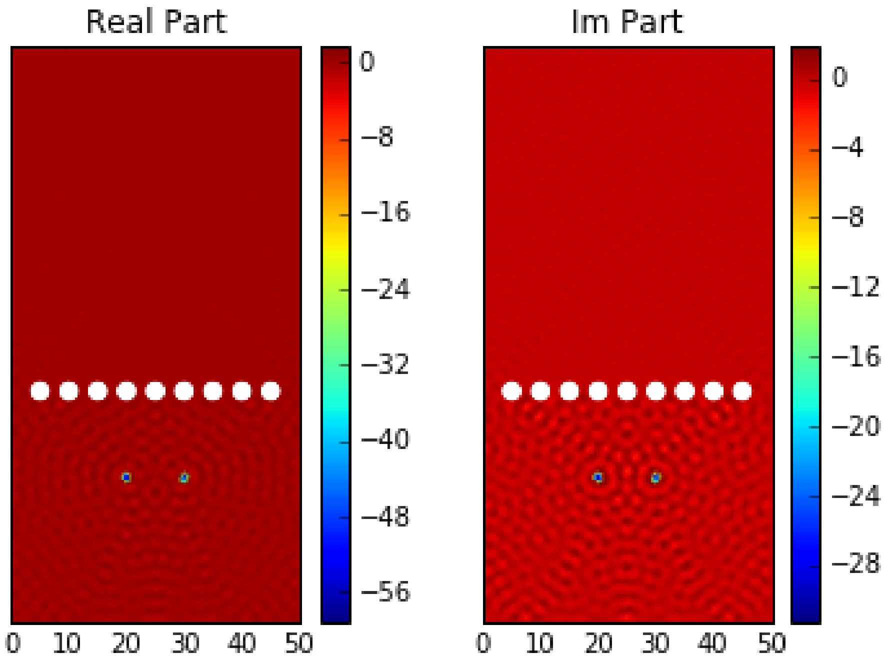


Figure 8: Here $\lambda = 1$, L = 100.

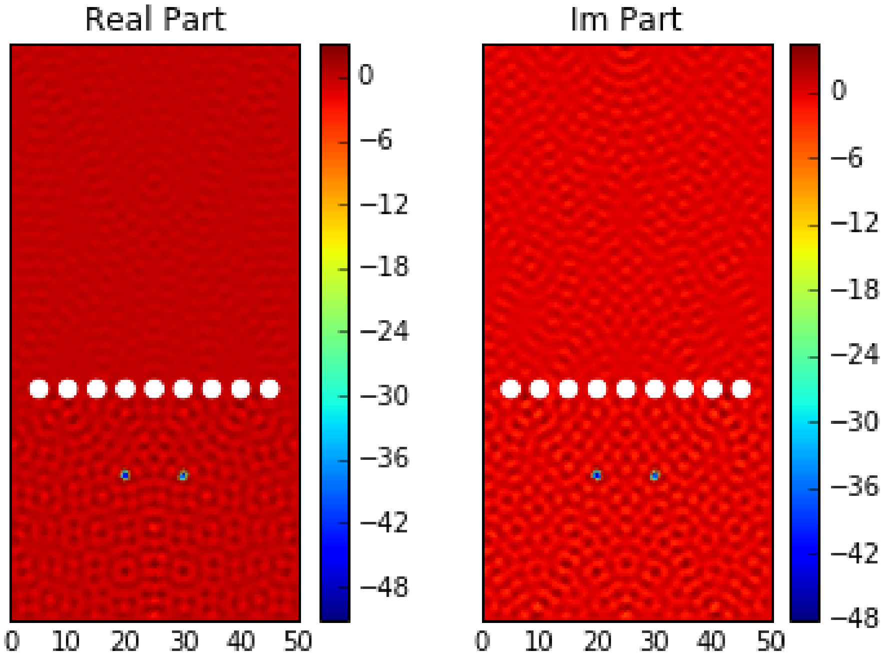
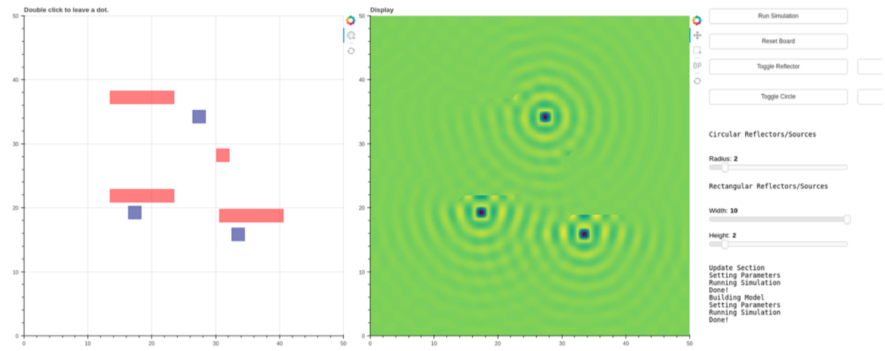


Figure 9: Here $\lambda = 1$, L = 1000.

4 Additional Features

We have also developed a Python API for running these simulations which is then interfaced through a Bokeh front end.



Circular Reflectors/Sources

Radius: 2

Rectangular Reflectors/Sources

Width: 10

Height: 2

```
Update Section
Setting Parameters
Running Simulation
Done!
Building Model
Setting Parameters
Running Simulation
Done!
```

Figure 10: Example of the interactive Bokeh application for running plasmon simulations. The red regions represent rectangular reflectors and the blue regions represent rectangular sources.

5 Conclusion

We were able to solve the plasmon wave equation in FEniCS and build an API to allow for the arbitrary creation of different samples with arbitrary placements of sources and reflectors. This API is then accessed by a Bokeh front end that provides an interactive way to simulate plasmons. This can be used to theoretically verify experimental results and further work will be done in making it more accurate by including other effects.

References

[1] A. S. Rodin, Z. Fei, A. S. McLeod, M. Wagner, A. H. C. Neto, M. M. Fogler, and D. N. Basov, “Plasmonic Hot Spots in Triangular Tapered Graphene Microcrystals,” no. 4, p. 4, 2013.