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Physics Major Reed Hodges: Blue Waters Student Internship Update

October 27, 2016



Reed Hodges coding at the National Center for Supercomputing Applications in Illinois

Last spring, Physics Major Reed Hodges received a prestigious NSF-funded Blue Waters Student Internship, which included spending two weeks at the Petascale Institute, at the National Center for Supercomputing Applications at the University of Illinois in Urbana-Champaign in May 2016.

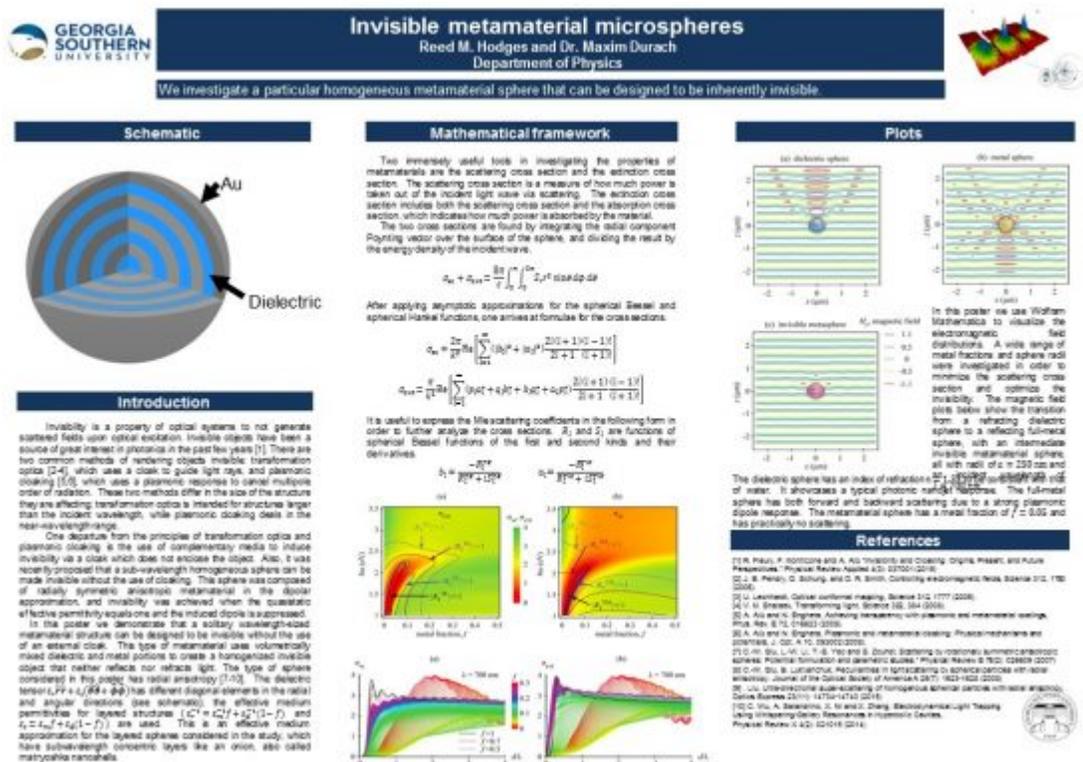
This year-long internship is hosted by Dr. Durach's group at Georgia Southern University. The work on the project involves two stages: (a) development of Mie theory codes, which will allow calculation of electromagnetic fields and scattering properties of spherical particles. (b) consideration of spherical particles coupled to planar interfaces and calculation of electromagnetic fields in such structures.

The first part of the project is complete. Mie theory codes were developed in Mathematica and Fortran and tested on metamaterial metal-dielectric spheres, for which fields and cross-sections can be calculated for arbitrary metal fractions from pure dielectric to pure metal reproducing results from the literature.

As an extremely pleasant and important by-product of this part of the project it was established that wavelength-scale metamaterial spheres with metal fractions $\sim 5\%$ exhibit invisibility. Previous work on invisibility invariably separated invisible objects into hidden and cloaking sections. In the invisibility scheme which we propose it is not possible to determine

what is cloak, since the object is a homogeneous sphere. Therefore our work opens up an important research direction in optics – invisibility without cloaking and demonstrates that this approach is possible in principle. The corresponding manuscript is written and is currently in the editing phase and soon will be submitted to a high-impact peer-refereed journal and to arxiv.

This work was submitted to Georgia Undergraduate Research Conference in Milledgeville, GA in the form of two posters (posters 1 and 2), in which the invisibility mechanism was described and the work in Mathematica and Fortran programming environments was compared. Both posters were accepted and one received an outstanding review, suggesting that the work should be presented as a talk. Reed Hodges and his collaborator Kelvin Rosado will travel to Milledgeville to present this work.



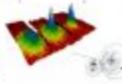
Poster 1. R. Hodges, M. Durach, Invisible Metamaterial Spheres

After the presentation, Dr. Durach and Reed we will turn to the second phase of the project.



Developing Fortran Codes for Photonics Research

Kelvin Rosado, Reed M. Hodges, and Dr. Maxim Durach
Department of Physics



We detail the development of a Fortran library used to plot quantities related to the scattering of dielectric spheres, and compare speed, efficiency, and results to those of Wolfram Mathematica.

Introduction

Different programming environments provide different advantages in scientific computing. The high-level symbolic computation of Wolfram Mathematica allows for less time-consuming and intuitive programming, and it has a variety of mathematical functions ready for use. This provides easier access into physics research for undergraduate students. Fortran, on the other hand, has a much more involved programming experience and does not contain nearly as many ready-to-use functions. However, Fortran may be more computationally efficient compared to Mathematica in some problems. In this study we compare the efficiency of our Fortran and Mathematica codes.

Plotting electromagnetic field distributions with photonics structures requires many individual computations, which suggests the use of high-performance computing. The fields interacting with wavelength-sized dielectric spheres are modeled via Mie theory, which treats them as infinite sums of vector spherical harmonics. The different mathematical functions involved include spherical Bessel and Hankel functions of the first kind, and associated Legendre polynomials. We developed a Fortran mathematical library to evaluate these functions and more. The library was then used to plot electromagnetic field distributions for light of different wavelengths, polarizations, and incidence angles, and for spheres of varying radius and permittivity. Scattering and extinction cross sections were plotted in order to analyze how power is taken out of the incident wave. The computation times of these codes is

Examples of code and speed comparisons

Our Fortran math library consisted of functions for associated Legendre polynomials, spherical Bessel functions, spherical Hankel functions, and their derivatives. The associated Legendre function used recursion to calculate polynomials of negative order m .

Figure 1 highlights the relative simplicity of Mathematica compared to Fortran in calculating spherical Bessel functions. Conversely, Table 1 contains the data that demonstrates Fortran's faster calculations. Mathematica can be anywhere from 1.6 to 25 times slower than Fortran for these particular functions.

```

Mathematica
In[1]:= BesselJ[0, 1]
Out[1]= 0.766261834744145
In[2]:= BesselJ[0, 1]
Out[2]= 0.766261834744145
In[3]:= BesselJ[0, 1]
Out[3]= 0.766261834744145
In[4]:= BesselJ[0, 1]
Out[4]= 0.766261834744145
In[5]:= BesselJ[0, 1]
Out[5]= 0.766261834744145
In[6]:= BesselJ[0, 1]
Out[6]= 0.766261834744145
In[7]:= BesselJ[0, 1]
Out[7]= 0.766261834744145
In[8]:= BesselJ[0, 1]
Out[8]= 0.766261834744145
In[9]:= BesselJ[0, 1]
Out[9]= 0.766261834744145
In[10]:= BesselJ[0, 1]
Out[10]= 0.766261834744145

```

```

Fortran
      REAL(8) :: BesselJ0
      BesselJ0 = 0.766261834744145
      PRINT *, BesselJ0
    
```

Plots

The Fortran math library is used in plotting electromagnetic fields and scattering cross sections. Some examples of such plots are given below. They show the structure of photonic resonances, which are areas of increased intensity on the back side of the sphere. They are the result of a lensing effect by the sphere, and have numerous applications in nanoscience. The scattering cross section plots show the varying of the cross section over the surface of the sphere. The shape of the plot agrees with that of the one predicted by the formula for the cross section developed by van de Hulst.



Fig. 1. A comparison between Fortran (left) and Mathematica (right) for the calculation of spherical Bessel functions. This is only half of the needed Fortran code, while the Mathematica code prints a list of 50 different values for the function.

	Fortran (avg. of 10 trials)	Mathematica (avg. of 10 trials)	Ratio
Extinction cross section (sum of 100)	1.076×10^{-10} s	4.821×10^{-10} s	18.78
Extinction cross section (sum of 1000)	1.076×10^{-10} s	4.871×10^{-10} s	18.27
Extinction cross section (sum of 10000)	1.076×10^{-10} s	2.467×10^{-10} s	2.487
H_{01} Coefficient (sum of 100)	1.108×10^{-10} s	8.424×10^{-10} s	24.64
H_{01} Coefficient (sum of 1000)	1.117×10^{-10} s	5.263×10^{-10} s	21.99
H_{01} Coefficient (sum of 10000)	1.076×10^{-10} s	4.661×10^{-10} s	11.67

Table 1. A comparison of run times for various functions in Fortran and Mathematica.

Mie theory and cross sections

Mie theory is the basis for the electromagnetic interactions between light and near-wavelength spherical objects. It expresses electromagnetic fields as infinite sums of vector spherical harmonics, one such function is

$$M_{lm}^{(1)} = \sqrt{\frac{4\pi}{3}} \left[r Y_l^m(\theta, \phi) - \frac{2m}{l(l+1)} \frac{Y_l^{m-1}(\theta, \phi)}{\sin \theta} \right]$$

The scalar potential $\psi_l^{(1)}$ is a solution to the scalar wave equation and has the general form below, where $z_l^{(1)}(kr)$ is either a spherical Bessel function or a spherical Hankel function, depending on the value of l .

$$\psi_l^{(1)} = z_l^{(1)}(kr) Y_l^m(\theta, \phi) e^{im\phi}$$

Within the sums that yield electromagnetic fields, these spherical harmonics have the so-called Mie coefficients. Their values are found by solving the boundary conditions at the surface of the sphere, the three components of the fields must match at the boundary.

Once the coefficients are known, the scattering cross section can be calculated. The formula for the cross section is found by integrating the radial component of the Poynting vector over the surface of the sphere, this process yields

$$\sigma_{sc} = \frac{4\pi}{k^2} \sum_{l=1}^{\infty} \sum_{m=-l}^l \left[|b_l^m|^2 + |c_l^m|^2 \right] \frac{l(l+1)}{2l+1} \frac{(l-1)!}{(l+1)!}$$

References

- [1] C. Wu, A. Salandrino, X. Ni, and X. Zhang, "Electrodynamical Light Trapping Using Whispering-Gallery Resonances in Hyperbolic Cavities," *Physical Review X* **4**, 021016 (2014).
- [2] O. Vildavsky, "Light scattering from a sphere on or near a surface," *Journal of the Optical Society of America A* **8**, 432 (1991).
- [3] J. A. Stratton, "Electromagnetic Theory," (IEEE Press, 2007).

Poster 2. K. Rosado, R. Hodges, M. Durach, Developing Fortran Codes for Photonics Research

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