

Personal Essay

Although my educational background is primarily in mathematics and computer science, I have always been interested in applying these areas to the sciences. While scientific computing has led to breakthroughs in many fields, I think the most exciting discoveries remain in understanding life at the molecular level. Through such understanding, it will be possible to understand and prevent genetic diseases, design drugs to fight them, and relieve suffering for people around the world. There are many exciting and useful applications of computers in molecular biology and chemistry, but they are all fundamentally limited by the tradeoff between the level of detail and size of simulations. In order to make further progress, new algorithmic ideas are necessary.

I intend to apply my background in applied mathematics and algorithm design to improving fundamental calculations in computational chemistry. In order to accomplish this, I am pursuing a Ph.D. in computer science at Georgia Tech. I am working in the Computational Science and Engineering Division and being advised by Alexander Gray and David Sherrill. I am able to work closely with faculty in both algorithm design and scientific computing. My eventual goal is to continue my research as a university professor.

1 Teaching

For five semesters as an undergraduate, I worked as a teaching assistant in the School of Mathematics for courses on linear algebra, calculus, and differential equations. I was responsible for grading tests and answering students questions. However, the part of the job I really enjoyed was teaching the recitation sections. Twice a week, I was responsible for leading a section of about 40 students for an hour. In general, the professors I worked for gave me few instructions, so I was free to organize the class as I saw fit.

I loved the challenge of communicating complex ideas to (often disinterested) students. I quickly came to appreciate the difficulty of this task. In order for any of them to stick, every concept had to be carefully motivated. Complex details had to be carefully summarized. Too many details, no matter how interesting I found them, quickly lost all of the students. Too few, and they were unable to handle subtle problems later. I found students were often best motivated by examples in applications. A student interested in computer graphics would doze through linear algebra until I motivated reflection of light as a matrix computation. Realizing the power of this method motivated me to learn more about these applications. I began bombarding friends in various fields for examples of eigenvectors and Laplace transforms in their classes. As I became more involved in my own research, I often used it as a source of examples.

2 FASTlab

In my last summer as an undergraduate, I started working with Alex Gray's research group, the FASTlab. Initially, I was researching a faster algorithm for finding Euclidean Minimum Spanning Trees. Although I had done research before, it was an individual project. Now, I found myself interacting with several graduate students with backgrounds in mathematics, sciences, and computer science, all working on fast algorithms for various applications.

Teamwork. I quickly learned to appreciate working with the other students. I was trying to apply some of the lab's previous work to a new problem. Before I could even begin,

I had to fully understand the published algorithms. I often sought out the other students with questions. When working on my own algorithm, I gained many valuable suggestions from the other students that helped me overcome difficulties. Even simple tasks like learning the lab's code base were much easier in a group environment.

Since my initial work with the FASTlab, my own research has expanded to include more scientific applications. Although I generally pursue my own projects, I rarely miss opportunities to discuss them with the other members of the lab. While investigating opportunities in computational chemistry, I realized I needed a better understanding of quantum mechanics. I did extensive reading on my own, but I often sought the help of the lab's physicist postdoc.

Communication. With the FASTlab, I have gained valuable experience in presenting my ideas to diverse audiences. Each week, a student gives a one hour talk on his or her research. I have presented on my work on minimum spanning trees and on some investigations in computational biology. Presenting the technical details involved in simulating protein folding was particularly challenging, given that the audience was mostly from a mathematics and computer science background.

Additionally, we are engaged in collaborations with several other research groups. We often give presentations on our work to other research groups, both in computer science and other sciences. We have presented to Prof. Jeffrey Skolnick's computational biology group and Prof. David Sherrill's computational chemistry group. On both occasions, I was responsible for preparing slides and presenting about my work and ideas, which involved communicating material from statistics and algorithm design to scientific audiences. Both of these meetings led to ongoing collaborations with these researchers.

3 Goals

After finishing my degree at Georgia Tech, I plan to continue my research as a university professor. While there are many ways to pursue research, I believe that academia offers the greatest freedom to impart my ideas to students and colleagues, interact with scientists, and ensure that my work has the greatest possible benefit. As a professor, I will also have the opportunity to continue teaching. In addition to the challenge this provides, I think it is an excellent opportunity to further solidify new ideas by presenting them convincingly to more than just experts.

At Georgia Tech, I have studied applied mathematics and sophisticated algorithms. I have been able to establish a network of collaborators to assist me in making meaningful applications of these ideas to chemistry and biology. I have gained valuable experience with communicating my ideas to a variety of audiences. All of these factors make it possible for me to make a significant contribution to these important fields. The NSF GRF would make it possible for me to continue applying my expertise to detailed and complex problems in the sciences without having to fit in to the funding of any single professor, thus freeing me to continue working with my broad range of collaborators.