

## **Research Statement**

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My research explores techniques in numerical analysis and scientific computing. I try to incorporate insights from numerical analysis, computer science, and other fields of mathematics to justify and implement approaches to novel models of physical processes. I intend to further this work through postdoctoral research touching on one or several of these themes.

My overall goal is to bridge the gap between fast numerical methods and important areas of application such as computational biochemistry and computational fluid dynamics. My approach is to use software automation in conjunction with fast solution methods in order to explore options for the solution of problems in a variety of application areas. I have focused on geometric multigrid methods for elliptic problems and computational biochemistry as areas of study and application. I focus on both on efficient and widely-applicable numerical methods and discretizations in conjunction with novel models for physical systems.

## **Research Experience**

My ongoing research projects tend to fall into either basic research in numerical methods or application of numerical methods to specific problem areas. These projects fall into the categories of fast numerical methods, bioelectrostatics, and automated scientific computing. These are all interrelated, but deserving of separate description.

### **Fast Numerical Methods**

I have studied, developed, and implemented methods for geometric unstructured multigrid. In particular I have focused on achieving textbook multigrid efficiency in the case of complex and highly graded meshes. Developing these methods requires being able to justify fast convergence of the solution based upon the quality of the coarse spaces, and requires in-depth study of the numerical analysis of multilevel methods and computational geometry. I am in the process of extending this work to the case of jump coefficients, anisotropic meshes, and nonlinear solvers.

I have also investigated fast methods for integral equations for problems in biological electrostatics. These include both fast and GPU-accelerated fourier-space methods, and methods using the relation between an operator and its Green's function. I am working on incorporating these methods into simulations of proteins and ion channels.

### **Bioelectrostatics**

I have been studying an array of models and formulations for solvation in protein biology. These problems span two major projects. The first of these projects involves studying and extending models for nonlocal permittivity effects on the solvation of small molecules. The novel approach taken by this project is that while the nonlocal term in the formulation

is easily stated as an integral equation, it is easily taken back to the framework of differential equations as well. I developed and implemented a finite element realization of this model for use in determining solvation properties of small molecules, and further extension of the software will allow investigation of larger molecules, such as proteins, under this framework. This work is in conjunction with Dexuan Xie at the University of Wisconsin at Milwaukee.

I have also worked on developing methods for the approximation of certain integral operators for classical density functional theory calculations. This work is in conjunction with Matthew Knepley and Dirk Gillespie at Rush Medical Center in Chicago. These calculations allow for the determination of ion concentrations around biomolecules where the effects of ion proximity are explicitly modeled, improving the accuracy for high-ion-concentration behavior of a reduced-model ion channel. My contribution to this project was to provide GPU-accelerated direct and fast approximate methods for calculating a screening effect in the model. This effort led to a several-hundred-times speedup of what was by far the most expensive part of this calculation. We able to explore this model numerically.

## **Automated Scientific Computing**

I have tried to incorporate the use and development of automated scientific computing methods and software into these projects as much as possible. I have been active with the FEniCS project, an international group of researchers working to build tools for the automated creation of finite element method-based calculation and simulation tools. I have used this code to build software for the calculation of quantities related to solvated proteins using different solvent models. I have also extended the solver and meshing interfaces of this project in order to enable unstructured geometric multigrid methods. I have added other features as well, including the technology necessary for the representation of isoparametric boundaries for use with bluff-body turbulent fluid simulations.

## **Research Agenda**

My graduate research experience prepared me for a variety of potential future directions. Interdisciplinary, inter-institutional and international research collaboration were highly emphasized in my graduate education. I have experience conducting research with a number of different types of groups in different parts of the world. These include experience as a scientific programmer with some research responsibilities and as a visiting researcher. I have been in both research lab and academic settings. The contacts and experience I have gained through this should allow me to be a more able researcher in the future.

An ideal position for me would have an exciting application that I could really focus on. Future postdoctoral research should lead to interesting problems that extend the research I have already started while furthering my education in numerical analysis. Such a position would allow me to continue gaining experience in scientific computing and gain insights that would allow me to become a successful future researcher.