

# Summary of Current Research Interests

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## Research Philosophy

Modeling is in the essence of human knowledge. We seem to understand nature better if we can devise models of the complicated phenomena that surround us. Mathematical modeling provides necessary abstractions convenient for describing, explaining, and predicting the behavior of different phenomena. In fact, mathematics has provided so many powerful intellectual tools that it has been recognized by many as the language of science and technology. Together with the mathematical modeling, simulation and data intensive computing have become staples of modern scientific life across nearly every domain and discipline. The dramatic improvements in computing and information technology over the past two decades have provided scientists with powerful tools for modeling and simulation. The complexity of these tools, however, has also been steadily increasing and the efficient application of scientific computing techniques continues to require constantly growing amounts of specialized knowledge in a variety of diverse scientific areas such as numerical analysis, algorithm theory, computer architectures, and programming languages. Throughout my research career, while working on different projects whose focus was usually on one of these areas, I was able to acquire a considerable experience in all of them. Currently, my main research goal is to use this experience in developing advanced new methods and tools for scientific computing.

## Current Research Projects

My main research interests are in the areas of applied mathematics and scientific computing. My current research focuses on fast algorithm development and efficient implementation on modern computer architectures. During my stay at the University of Houston, Department of Computer Science I have been fortunate to have the opportunity to work on a wide variety of projects and to collaborate with many prominent researchers. Here is a brief description of projects that I am currently working on.

## Scientific Software Libraries – UHFFT

The main goal of this project is development and implementation of a portable and efficient software library for fast Fourier transforms. The library should adapt easily to a new and advanced hardware and to the application software as well. To achieve this goal a completely new approach to the library software development was needed in which the main effort so far has been devoted to the construction of tools and infrastructure for automatic code generation and optimization. As a final result we have developed a library that adapts automatically to the hardware it is running on by using a dynamic construction of the FFT algorithm. This is accomplished through the selection of the fastest combination of composable blocks of code called codelets which are generated and optimized for the underlying architecture during the installation of the library. We have also developed an efficient automatic method of generating and optimizing the library modules by using a special-purpose compiler. The code generator is written in C and it generates a library of C codelets. The code generator is shown to be flexible and extensible and the entire library can be (re)generated in a matter of seconds. The major novelty in the library is that most of the code is automatically generated during the installation of the library with an attempt to tune the installation to the particular architecture.

The adaptive approach we use is also compatible with the methodology of the GrADS project (see below) in which the complexity of the grid architecture requires software designed to support adaptation and performance monitoring. UHFFT is also part of the Self Adaptive Numerical Software (SANS) project. SANS is a collaborative effort between different projects that deal with challenges in development of the intelligent next generation numerical software.

This work has been carried out with partial support from the DOE funded Los Alamos Computer Science Institute (LACSI), the GrADS project funded under the Next Generation Software initiative with the National Science Foundation, and in part by the Alliance funded as part of the NSF PACI program.

## Grid Application Development Software (GrADS)

The Grid Application Development Software (GrADS) project is a collaborative effort sponsored by the Next Generation Software (NGS) program of the National Science Foundation. The institutions involved include Rice University, University of California San Diego, University of Tennessee, Uni-

versity of Chicago, University Southern California-ISI, University Illinois at Urbana-Champaign, and University of Houston. The goal of the GrADS project is to simplify distributed heterogeneous computing so that the global information infrastructure (the Grid) can be used in a qualitatively different way—as a computational as well as an information resource. There are many scientific and technical problems that must be solved to make it easier for ordinary scientific users to develop, execute, and tune applications on the computational grid that connects the nation's computers, databases, and instruments. My efforts in the GrADS project are related to the development and integration of numerical libraries in the grid environment, in which computing resources are distributed, heterogeneous, and dynamic. The GrADSoft architecture requires configurable applications that can be optimized at runtime for execution on a specific collection of Grid resources. The use performance monitoring is needed for adaptive tuning of applications to the constantly changing environment. The adaptive approach developed in the UHFFT library already satisfies most of these requirements and my current research focuses on the deployment and integration of the UHFFT library into several test applications.

### **Image Reconstruction in Electron Microscopy (EM)**

This project is a collaborative effort between the National Center for Macromolecular Imaging (NCMI) at Baylor College of Medicine and the University of Houston. The goal of this project is to establish the computational infrastructure for fast, routine, atomic structure determination of subcellular complexes using a sophisticated computer reconstruction of images generated in the electron cryo-microscopy. The reconstruction produces three-dimensional images that can be used for design of drugs and vaccines for a variety of diseases. Low dose electron images have a very low signal-to-noise ratio and a large number of single particle images ( $10^3 - 10^6$ ) is needed for the full 3-D reconstruction of various macromolecular machines. This process is both data and computation intensive and requires a number of image processing steps on terabyte-scale datasets. My research in this project is related to the development and implementation of efficient algorithms for 3-D image reconstruction and analysis. This involves the extensions of the UHFFT adaptive methods to the various signal and image processing routines used in the reconstruction process. The complete reconstruction procedure involves, usually, the instrument and a variety of storage, computational and visualization resources. Since these resource are, in general, distributed the reconstruction procedure was recognized as one that could

benefit considerably from using the GrADS infrastructure. I am currently working on the implementation of various EM reconstruction procedures in the GrADS environment.

## Hemodynamics Modeling and Simulations

Since 1999 I have been investigating hemodynamics flows with colleagues at the University of Houston, University of Texas, Austin, University of Lyon, and Texas Heart Institute. We are developing mathematical models and software that will provide physicians and biomedical researchers with a fully automated simulation-based approach to quantifying the hemodynamics in the human vascular system and in various vascular prosthetic devices. The goal of this project is to make patient-specific hemodynamic simulation results available to medical professionals in a concise and usable format as an aid in treatment planning.

One particular problem we have been working on is the modeling and simulation of endovascular repair of the abdominal aortic aneurysm (AAA). Aneurysm is characterized by the formation of sac-like protrusions of weakened sections of blood vessels that can rupture and be fatal. Within the past ten years an innovative non-invasive procedure, which requires only local anesthesia, has been developed. The new procedure entails inserting a catheter (a hollow tube) into an artery and directing it to the site of the aneurysm. Placed in the catheter is a spring-like device called a stent, which serves to hold open the weakened artery and to exclude the aneurysm from circulation. This lowers the probability of rupture and promotes aneurysm shrinking due to thrombosis caused by the lack of blood supply to the aneurysm tissue. The modeling and simulation approach we take has several levels. At the first level we develop a simplified, one-dimensional model of blood flow thorough an axisymmetric, elastic tube (blood vessel and/or stent) to detect scenarios in which complications occur. At the second level we study these scenarios in detail by considering a three-dimensional model. At the third level we plan to perform a validation of the modeling assumptions through the comparison with in vivo/in vitro measurements. My contribution to this project is in modeling and simulation of blood vessels after endovascular repair in order to predict and evaluate the consequences of different treatment options. Preliminary analysis of the one-dimensional model together with the results obtained from the numerical simulations, already suggest an improvement in the design of stents and in the procedure planning.

## Fast Methods in Computational Chemistry

In 2002 I started a project with Prof. M. Pettitt at University of Houston on development and implementation of numerical methods for fast evaluation of Coulomb potentials and forces in molecular dynamics simulations. The limiting computation in all N-body problems is the evaluation of potentials and forces between all pair-wise combinations of particles. The significant acceleration can be obtained by using the Greengard-Rokhlin Fast Multipole Algorithm which aggregates the effects of distant particles into a series expansion, and reduces the computational complexity by interacting particles with these aggregates rather than computing all pairs. Further improvements can be obtained by using the fast Fourier transform for computation of a convolution-like operation on a matrix of multipole coefficients. My research related to this project is two-fold. The first part involves the analysis of different sparse factorization and decomposition procedures with respect to the computational efficiency and stability. The second part involves the use of the code generation and optimization infrastructure developed in the UHFFT library for architecture dependent automatic performance tuning of these procedures.

## 1 Summary of Past Research Projects

My first research experience came during my work in the Department of Energy at the University of Zagreb, Croatia, where I was working on numerical simulation of thermal-hydraulic phenomena in nuclear reactors. In my master's degree thesis, I used a finite volume approximation to solve a system of conservation laws describing two phase flow in a nuclear reactor core. I applied this model to simulate a variety of nuclear safety related transients. I continued my work in the same area in the Department of Nuclear Energy at Brookhaven National Laboratory, where I was appointed as a visiting scientist under an International Atomic Energy Agency fellowship. During that period I gained a valuable experience in numerical modeling of real-life engineering problems.

In my PhD thesis I implemented an efficient parallel algorithm for the mixed finite element approximation of the second order elliptic problem. By using a non-overlapping domain decomposition approach I have replaced the original problem by a set of independent subdomain problems and a global interface problem. I have introduced an efficient preconditioning method which has significantly improved the convergence rate of the conjugate gradient method used to solve the interface problem. This algorithm was used

for the solution of computationally intensive problems arising in simulations of the multiphase flow in the porous media.

While at Iowa State University, I have developed and implemented a general N-dimensional finite element package for numerical approximation of partial differential equations. All the routines in the package have been developed in an innovative recursive way, such that both the dimension and the order of the FEM approximation can be specified as input parameters. This code has been instrumental in numerical approximation of the multidimensional Fokker-Planck equation whose solution is an important integral part of many challenging problems in science and engineering. The development of the code was driven by the need to solve a nonlinear stochastic filtering problem arising in the multitarget tracking problems (supported by ONR) and modeling of laser cooling problems.