Department of Scientific Computing

Summer 2018

CONTENTS

Shanbhag group excels with science & scholarship

Trained as a chemical engineer, Scientific Computing's resident polymer scientist, Sachin Shanbhag, does research in a very contained, but critical area of computational materials science. In particular, Shanbhag is part of a small group of scientists who study polymer dynamics, a tiny, but complex part of materials science that seeks to understand and predict how polymers move under certain conditions such as heat, stress, or shear.

From a historical viewpoint, computational polymer science has evolved over the years. Beginning in the mid-1850s, polymer science resembled a practice or art; a century or so later, just as computers emerged as a common tool for scientists, the field was dominated by engineers and chemists who were interested in synthetic polymer materials applications such as Bakelite. Later, around the mid-1930s, the interesting properties of these materials enticed scientists who developed quantitative theories to link the structure and properties of polymers. Not long thereafter, these theories became too difficult to solve analytically. As computing power became available, polymers were among the first materials to be studied using Monte Carlo methods. Polymer dynamics, Shanbhag's chosen research area, benefits greatly from computation and computational modeling. In fact, Shanbhag's sophisticated, computation-rich research would not be possible without high performance computing.

"Research is fun when the underlying problem is either interesting or important. Polymer science is both; endless fascination from a scientific standpoint, and extremely important from a commercial standpoint," said Shanbhag.

To advance his scholarship, recently Shanbhag was awarded a three-year, $250,000 National Science Foundation grant to study condensed matter and materials theory by exploring the development of augmented tube models and to test these augmented models on the computationally intensive inverse problem of inferring the composition of a polymer mixture from experimental measurements of rheology. The project seeks to combine the strength of tube models with that of slip link models for studying entangled polymer melts. Slip link models tend to be successful, but computationally costly, for studying entangled polymer melts, while tube models tend to consistently fail even for relatively simple systems like binary blends of monodisperse polymers with widely separated relaxation times. If Shanbhag's project is successful, the new model can be a template for other problems in materials science that seek to combine a mean-field theory with simple simulation models.

Professor Sachin Shanbhag

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In addition to his ongoing scholarship, Shanbhag assists students and contributes to the department administratively, currently serving as mentor for his students and graduate program director for all the department's grad students. As graduate program director, Shanbhag helps masters and doctoral students navigate the graduate degree process. In one of his most important tasks in that role, he facilitates and coordinates preliminary examinations for those students who have completed appropriate coursework, and are ready to move to candidacy and their own individual scholarship.

Shanbhag assists students in other roles. He has mentored or supported over 40 students at all levels since 2006 when he arrived at the department, including undergraduate honors thesis writers, masters degree students in Engineering and Scientific Computing and most recently, his own doctoral students Benjamin Crysup and Eitan Lees.

Crysup joined the Department of Scientific Computing in 2008 as an undergraduate student, then continued in the department after completing his studies in computational science, moving to the Ph.D. program in 2013. Before graduating in 2017 with his doctorate, Crysup racked up an extensive list of accomplishments as a student, using a broad set of academic and technical skills. Often, Crysup went well beyond what was required using his intellect, curiosity and ingenuity to create physical and technical models, mentor Young Scholars Program students, and research scholarly topics.

Benjamin Crysup

Eitan Lees

Shanbhag is especially impressed with the way Crysup provided mentorship and guidance to Alexandra Saavedra and Daniel Martin – two YSP students who spent a summer doing research in the Shanbhag lab. "Ben did all the hard work," said Shanbhag. "He was with them throughout the process of learning the ropes, crunching out the numbers. I stepped in occasionally to help make sense of the results; but this was mostly Ben's show." Crysup saw the students from start to finish on six-week projects with similar topics. Their research poster presentations focused on getting a good handle on how to deal with uncertainty in molecular simulations of particle trajectories using statistical methods.

With Shanbhag's assistance, another Ph.D. student is progressing through the pipeline toward degree and career success. Eitan Lees, a doctoral candidate studying with Shanbhag, has completed coursework, passed comprehensive exams and been admitted to candidacy. While writing his dissertation, Lees has continued to present nationally; this past June he gave a workshop at the Massachusetts Institute of Technology on his research, "Electroneutrality constraints in nonlocal models." Lees taught Introduction to Scientific Computing for the first time during the summer as well.

Overall, Shanbhag's continuous, broad contribution to Scientific Computing, students and scholarship have left him well regarded in the department, in Arts & Sciences and in the rheology community. By using computational tools, algorithms and simulations to advance research, and by dedicating his time and individual attention to students and the department, Shanbhag has demonstrated the capability to shine in the full professorial complement of teaching, research, and community service.

For more, search on Sachin Shanbhag at www.geoset.info.
Find additional information at http://people.sc.fsu.edu/~sshanbhag/

SC grantee to study biological cell modeling

The National Science Foundation will support a new research project in the Department of Scientific Computing. Associate Professor Xiaoqiang Wang has been awarded

$100,000 for his project entitled, Energetic Phase-Field Methods and Biological Cell Modeling. The three-year project is scheduled for the period August 15, 2018 through August 14, 2021.

The funded work will be a continuation of Wang's studies in phase-field modeling. The phase-field model is a method of describing temporal microstructure evolution. It has been extensively applied to modeling in materials science [for such uses as grain growth and coarsening, crack propagation, and stress induced pattern formation], imaging and video processing, graphics, and scientific visualization. Along with the model's still growing applications, Wang and colleagues have made significant progress by applying the phase-field method to the study and analysis of cells and cell structures.

In the past, Wang has used phase-field models to study the behavior of cellular adhesions, cell fluid dynamics, and actomyosin driven cell oscillations. The group has modeled and simulated adhesion of cell membranes to substrate, cell-to-cell adhesions, vesicle and blood cell fluctuations in fluid fields. In addition, Wang and his collaborators derived a phase-field formulation to describe elastic bending energy. While these NSF-funded studies have increased in complexity, sophistication, and depth, Wang's advances in the methodology have caused a simultaneous increase in computational robustness and computational efficiency.

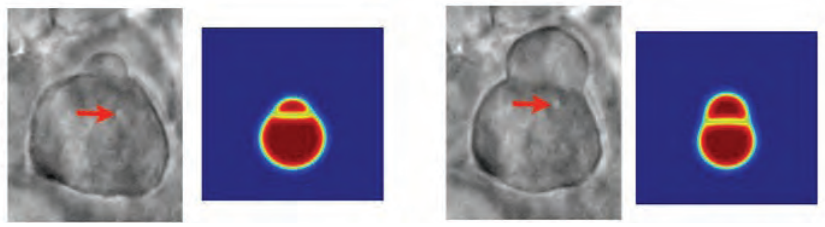
In the current project, Wang aims to develop efficient and reliable algorithms that have the potential to decrease computational costs, and facilitate an increase in the use of the phase-field method in solving moving boundary problems, including a complex biological system with multi micro-structures. Over the course of the grant, the research goals are:

1) development and analysis of a general framework using the augmented Lagrangian method for solving gradient flows with predefined parameters;
2) theoretical analysis of the exponential time difference Runge-Kutta method for solving the phase field equations;
3) coupling of the adaptive multigrid mesh with the exponential time difference schemes;
4) modeling the embedding and distribution of membrane proteins on a cell membrane;
5) modeling the interaction between a cell membrane and cytoskeleton, including cell blebbing, cell cytokinesis during mitosis and cell movement; and
6) modeling epithelial morphogenesis in Drosophila oogenesis.

The group also plans to improve previously developed phase-field model software. Enhancing the software in use will assist scientists by simulating the evolution and interaction of biological cells, and spur theoretical and practical applications for future research.

For more on Wang and his research, go to sc.fsu.edu.

For more on the National Science Foundation, go to nsf.gov.



Figures above, right and left. Comparison and preliminary result of Wang's cell blebbing[1] with laboratory observations of cell blebbing of a zebrash primordial germ cell. Wang and collaborators use this cell blebbing model to carry out multiple simulations in different biological processes. Observations show that the cell blebbing participates in the process of cell motility during cancer migration. By using this model, scientists can simulate cancer cells moving through the ECM, which helps them learn more about the conditions under which tumors spread. Blebs have been found in apoptosis, which is an important process during tissue development and virus response. By simulating bleb formation and the apoptotic bodies evolved by blebs, researchers can better understand these crucial processes.

[1] In cell biology, a bleb is a bulge, or protrusion of the plasma membrane of a cell, human bioparticulate or abscess with an internal environment similar to that of a simple cell, characterized by a spherical, bulky morphology. *Source, Wikipedia.*

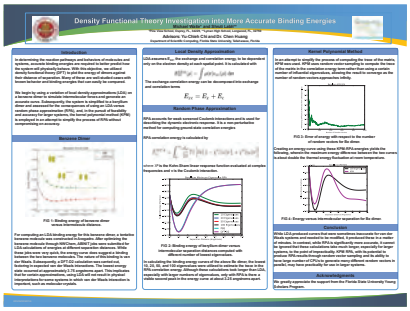
Huang, Smith take on Young Scholars

Above: Ph.D. candidate Danial Smith teaching a course to the Young Scholars Program students this summer. Smith taught Scientific Computing with C++, which focuses on the core principles of computing. The primary objective in the course is to convey the underlying principles involved in programming so students understand how to learn independently by exploring new languages, new libraries, new algorithms, and more. To that end, Smith tailored the class to be highly dynamic, immersive and intuitive. From the very first day of class, the students got their hands dirty, and after understanding the purpose behind the programs, they used specific examples to demonstrate functionality, methods and applications. This approach helped the students see the big picture through coding, examples, computation and fun.

At right, a reproduction of the research poster presented by Shruti Labh and Michael Waite, students mentored by SC assistant professor Chen Huang with assistance from SC grad student Yu-Chieh Chi. Labh is from Longwood, FL where she attends Lyman High; Waite, a student at Pine View School, is from Osprey, FL. Labh and Waite worked on computing the van der Waals interaction between atoms using the kernel polynomial method.

The Young Scholars Program (YSP) is a six-week residential science and mathematics summer program for Florida high school students with significant potential for careers in the fields of science, technology, engineering, and mathematics.

For more, go to:
facebook.com/fsuyoungscholars/



Above: 2018 Young Scholars Program participants pose for a group photo after presenting their research. Scientific Computing scholars supervised by Chen Huang are Shruti Labh [row one, first on left] and Michael Waite [row 2, end].

Bishnu accepts LANL research project

This summer began a year-long research project at a national laboratory for Scientific Computing (SC) Ph.D. student, Siddhartha Bishnu. The position is at Los Alamos National Laboratory (LANL), a US Department of Energy lab northwest of Santa Fe, New Mexico. "I will be working on a project at the Los Alamos National Laboratory this summer, during which time I will be supervised by Mark Petersen at LANL. In the Fall semester, the project will continue, and I will be co-supervised by Bryan Quaife from our department," Bishnu said.

This opportunity came in the second in as many years for the doctoral candidate. In summer 2017, along with fellow graduate student Shane Fogerty (University of Rochester), Bishnu examined approximate approaches for a range of DOE-specific computational problems run on a variety of architectures during a 10-week long Parallel Computing Summer Research Internship at LANL. Their research shows improvements in computational and memory performance, as well as in power savings. It also assesses application correctness while operating under the conditions of reduced precision. Their investigation uses computing estimates to address many of the identified challenges for exascale computing, leading to performance improvements that may include changes in fidelity of calculation.

Towards the end of the summer, two good things happened for Bishnu. First, he, along with Fogerty and their LANL mentors, Bob Robey, Laura Monroe and Joseph Schoonover, published and presented their work, "Thoughtful Precision in Mini-Apps" at the 2017 IEEE International Conference on Cluster Computing. The second thing that happened is that Bishnu was introduced to other scientists, including Mark Petersen, who studies geophysical and astrophysical flows at Los Alamos. Robey introduced Bishnu to Petersen during the final days of the 10-week project.

"On the last couple of days, Bob and Hai Ah (two of my mentors) introduced me to a few scientists at LANL. I realized that my research interests were most aligned with Mark Petersen. By then, I had already graduated with a MS in Applied & Computational Mathematics from FSU in Summer 2016 and was going to graduate with my second MS in Physical Oceanography in Fall 2017. Mark, who himself had graduated with two MS degrees before his Ph.D., liked my background and we discussed a future project where I would be working with him. Afterwards, he and two other scientists, Philip Wolfram and Xylar Asay-Davis, provided me with a few project options. I finally opted to work on Mark's project involving the improvement of the time stepping algorithm of the MPAS (Model for Prediction Across Scales) ocean model of LANL."

Bishnu's Scientific Computing mentor knows the importance of networking and contacts in an academic environments. "Internships, conferences, and presentations expose students' research to potential collaborators, Ph.D. advisors, and employers. Sid's research direction is a consequence of his diverse training and hard work. This opportunity shows why it is important to network and present your research whenever possible," commented Quaife.

Bishnu is curious about many different fields of science. His graduate studies

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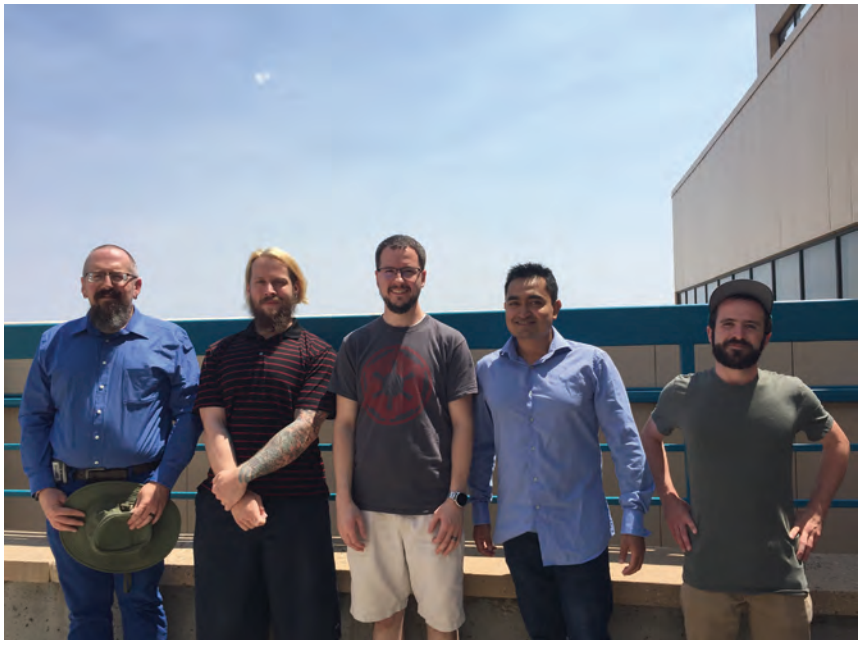


Above - SC @ LANL. From left: Geoff Womeldorff, Chad Sockwell, Doug Jacobsen, Siddhartha Bishnu, & Ezra Brooker.

Alum uses dissertation research to help launch nonprofit for international public education

While she was still a doctoral candidate, Haleh Ashki became aware of an acute need in her home country to educate people about sexual health. She wanted to address the issue through research that vast audiences – not just scientists - could understand. "People don't openly talk about sex and sexually transmitted diseases where I am from. These topics are taboo in Iran," Ashki said. "Sometimes journal articles and academic research are difficult to understand because they're written in a way that assumes a base knowledge about the subject. They focus solely on the new information their research brings to supplement that base. But I want as many people as possible to be able to understand."

When it was time, her skills and interests led her to select a dissertation that focused on the spread and dynamics of infectious disease; she modeled the progress of an epidemic in large populations by grouping individuals into three groups and discussed the role of contact network, disease transmission, recovery rate and preventive care. She liked the math, it was a phylogentic tree project, and her mathematics and biology backgrounds attracted her to Peter Beerli, Scientific Computing's resident phylogeneticist.

From the beginning, Ashki understood how intense the research would be. "I worked for an entire summer on finding information and educating myself. It wasn't Peter's research area at all, so I was really on my own. Luckily, there were people from other areas who were working on the subject. For example, there were faculty and students in mathematics who were working on the subject from a financial or cost viewpoint, or public policy affiliates were using a public health perspective. I focused my research on math and epidemiology, and essentially tried to combine Peter's epidemiology methods with my knowledge of the subject. As I progressed with my study, Peter and I educated each other."

Although writing her dissertation on the epidemic networks was satisfying, Ashki had a much larger long-term goal – getting reliable, accurate, accessible sexual health information to anyone in Iran who wanted it, while keeping confidentiality in tact. To that end, she and a group of close associates decided that starting a nonprofit whose mission is to educate the public in Iran would be the best approach for accomplishing their goal. As a group, they started Resources and Aid for Humanity, or the RAH Foundation. "RAH started with my sister, myself and some of my friends wanting to help women with sexually transmitted diseases in Iran. We decided to create a website and other computer-based tools to provide medical education and outreach."

The RAH Foundation is a small, but growing international nonprofit organization with no religious or political affiliations. It is committed to improve the health of individuals in the MENA (Middle East and North Africa) region by conducting education and awareness programs, building human resource capacities, and providing healthcare in the region.

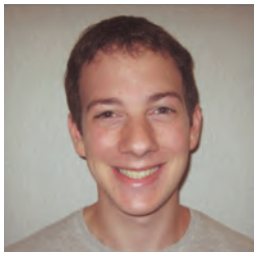
First, the foundation created a Facebook page, then launched a website in Farsi. "We started our project with a page on Facebook because it was an easy way for us to begin immediately. I wasn't physically in California at first, but was able to contribute to the organization by building the website and making educational videos." Today, in addition to the Facebook page, the foundation has websites in English and Farsi, one of the Indo-European languages primarily spoken in Iran, Afghanistan, and Tajikistan.

After the website was live, the foundation was interested in a creating a database that people could turn to that contained a bank of questions and answers. "We wanted people to have a good source of reliable information written in Farsi. We wanted to focus on sexual health, and include information people are shy about asking others. The explicit nature of the questions makes people less likely to come forward even though they may need the information very badly." To facilitate this in a way that provided accurate, reliable information, the foundation has a corps of physicians who quickly and anonymously respond to questions.

Since the beginning, there has been large scale interest in and interaction with the tools RAH created, signaling

Recent grads land positions in academia, research, & industry




A record number of doctoral candidates completed the Ph.D. during the summer. Five Scientific Computing students completed the degree during the summer term, marking an end to their studies at FSU. Amirhessam Tahmassebi, Michael Schneier, Lukas Bystricky, Ryan Learn and Philip Boehner successfully defended their dissertations in July.

Phil Boehner accepted a position at General Motors in Austin, Texas after defending his dissertation entitled, *Computational Framework for Evolution and Nucleosynthesis Studies of Astrophysical Objects*. Boehner will be helping to develop GM's finite volume-based PDE software package.

Lukas Bystricky packed up and headed to Vancouver right after completing his degree. Bystricky defended his dissertation, *Contact-free Simulations of Rigid Particle Suspensions Using Boundary Integral Equations*. In September, he will move to Switzerland to begin a postdoctoral position at KTH in Stockholm, Sweden. Bystricky will work in the numerical analysis group for Ana-Karin Tornberg on the multiscale modeling of viscous flows over rough/porous surfaces.

Ryan Learn successfully defended his dissertation, *On Some Multiphysics Effects of the Kelvin-Helmholtz Instability in Dense Plasmas*, on Monday, July 16, 2018. Learn's research was supervised by professor and astrophysicist Tomek Plewa. Learn accepted a faculty post at Washington State Univesity Tri-Cities, located in northern Richland, one of three regional campuses for Washington State University. In the fall, Learn will teach three courses -- linear algebra, engineeering statistics and introductory mathematics.

Michael Schneier defended his dissertation entitled, "*An Ensemble-Proper Orthogonal Decomposition Method for the Incompressible Navier Stokes Equation*." Schneier accepted a postdoctoral associate position at the University of Pittsburgh doing research in numerical analysis and uncertainty quantification.

After defending his dissertation, P*attern Recognition in Medical Imaging: Supervised Learning of MRI and fMRI Data,* and going through various interviews, Amirhessam Tahmassebi is deciding among job offers.

Ash Mechtley completed doctoral degree requirements in Spring 2018, relocated to Denver, and is working at the University of Colorado as a software engineer. Mechtley's dissertation is entitled, *Utilities for Off-target DNA Mining in Non-model Organisms and Querying for Phylogenetic Patterns*.

For more, go to sc.fsu.edu.

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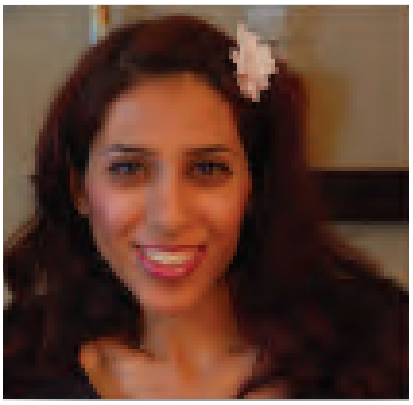
an enormous pent-up need for information within the community. The organization has focused on information that sharply reduces or removes a critical information void. "So far, we have educated more than 5,000 persons in workshops and have answered over 3,000 sexual health-related questions. We have trained 30 peer educators and have over 50,000 followers on social media," said Ashki. "Our focus is on women, information about sexual awareness, birth control – these things are essential. It is critical that women control their sexual health and sexual choices."

Haleh Ashki, Ph.D. is Director, Monitoring and Evaluation at RAH Foundation. For more on the foundation and their most recent endeavors, go to rah-foundation.org and GhayemBaShak.com.

To see a TEDx video about the foundation, its goals, reception and impact, go to https://youtu.be/HkzvDD0XfXE.



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Ph.D. student Siddhartha Bishnu

truly embrace the interdisciplinary aspects of science and computation, and his expansive interests are reflected in the wide-ranging science courses he studies. "I think I got this opportunity only because of my previous background. I had taken over 20 courses spanning four departments (Mathematics, Geophysical Fluid Dynamics Institute, Earth, Ocean & Atmospheric Sciences and Scientific Computing) which not only consolidated my basic concepts but also provided me with the tools to solve hardcore problems in math, physics and computing."

In late May, following his written comprehensive exams, Bishnu relocated to LANL; he plans to sit for the oral portion of the test in the Fall 2018 term. This scheduling freed him to concentrate his physical and mental energies on packing and getting relocated to New Mexico. Just a week or so after sitting for written prelims, Bishnu and his 15-year-old station wagon arrived safely in Los Alamos. "Much to the amazement of some of my friends, my 2003 Ford Focus and I survived the entire trip, and I picked up [fellow SC grad student] Ezra [Brooker] from the Los Alamos bus terminal when he arrived for his internship."

Since arriving at FSU for his grad studies, Bishnu has been on a path that helped him prepare for this research opportunity. He can see how his skills have developed over time and the many things he has learned that have helped him along the way. "When I first came to FSU, I could not code a simple program with confidence. The courses and professors [Shanbhag, Quaife, and Plewa among others] introduced us to a lot of tactics to make our graduate and future life easier and provided us with the guidance and directions to look for internships, job search, etc. These, I think, are very important to know in addition to our formal academic training. It is very helpful to assess our options beforehand and be prepared accordingly."

For more, go to lanl.gov.

www.sc.fsu.edu