Spring 2018

Department of Scientific Computing

Huang receives NSF CAREER Award

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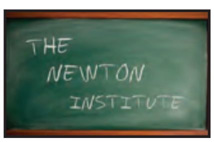
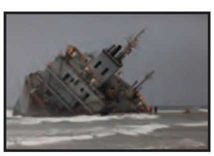
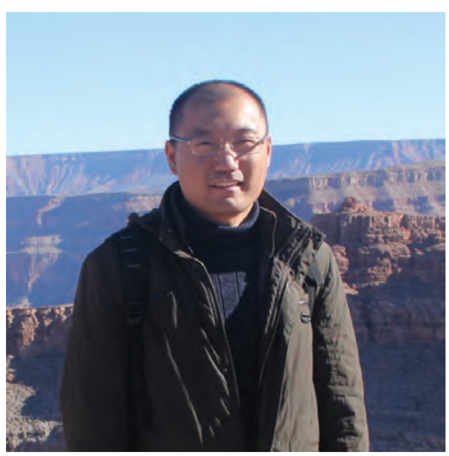




Dr. Chen Huang, assistant professor of computational science, received the National Science Foundation Faculty Early Career Development (CAREER) Award, a prestigious accolade intended to help kick-start the careers of promising junior faculty members.

Huang's proposal, titled "Local Correlation Approaches for High-Level Density Functional Theory Simulations of Large Systems" will be funded over the next five years through the Chemical Theory, Models and Computational Methods program in the Chemistry Division. "This NSF award will support my group to continue developing new methods for understanding and predicting electronic properties of materials at nanoscale. One project is to develop a new method to obtain reliable electronic structures at oxide interfaces. These interfaces are promising building blocks for designing high-performance electronic devices. Reliable predictions of their electronic properties are essential to accelerate the design of these devices," said Huang.



Assistant Professor & NSF CAREER Award winner, Chen Huang

The CAREER award will help Huang's group develop new methods to investigate electronic properties of large, complex molecules and material. Large systems are often needed for meaningful modeling, however, it is challenging to investigate large systems with highly accurate electronic structure methods, since their computational cost usually grows exponentially with system sizes. Huang and his group solve the electronic properties of large systems in a divide-and-conquer manner with the aim of overcoming this length-scale limitation. By incorporating these new methods, modeling of large systems is possible, therefore facilitating the discovery of novel materials necessary for advancing current technologies, such as resolving mechanisms of heterogeneous catalysis and novel electronic structures at oxide interfaces.

Huang is building an effective learning environment at FSU, training a diverse group of graduate students to investigate molecular and material properties using first-principle simulations. A problem-based density functional theory (DFT) course is being created with the goal of

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Sabbatical research focuses on collaboration and consultation

Xiaoqiang Wang, an associate professor in Scientific Computing, was awarded a sabbatical for the Spring 2018 semester. Wang, a faculty member at the department since 2006, studies the application of computational techniques to bioinformatics, computational neuroscience and similar biological fields. Wang's research uses numerical analysis and applied partial differential equations with applications to biology, scientific visualization, data mining, and fluid mechanics.

Wang introduced Edge Weighted Centroidal Voronoi Tessellations to the field, an important technique and method that can be applied to image processing, computer vision, data mining, and scientific visualization. His most recent scholarship has focused on modeling and simulation of cell membranes.

Sabbatical applications typically ask for time away from teaching to work on a specified research project – pure theory, a textbook, or preparing new courses. In a departure from the typical sabbatical request, Wang sought time to focus on collaboration with scholars and colleagues as a means to increase the scope, reach, and depth of his own research, and to inform the research of others.

"From the sabbatical, I was seeking new research directions," said Wang, "and looking for ways to spark new ideas. I wanted to share my research ideas with scholars and colleagues, giving them insight into what researchers at FSU were doing.

"Also, I am always looking for good potential students to introduce to our department. I wanted to inform the students about the research we have been doing, so those most interested could apply to our department."

The idea for these extended collaborations came to Wang years ago, influenced by time spent in China during the summer, and conceptualized as an extension of work he did with others. Wang had a short visit with Chengjian Zhang in June, 2016 while in Beijing doing research. At that time, the two discovered a large overlap in their research and discussed possible extensions of research topics and methodologies. Wang found Zhang's work on the Runge-Kutta method of special interest, as this method can be applied to Wang's own mathematical models.

Xiaoqiang Wang (right) assists students after a lecture.

During that time, Wang introduced Zhang's research groups to his scholarship on cell membranes by giving a talk and workshop on the subject. After Wang's presentation, the students expressed high interest in getting deeper into the work, systematically studying Wang's research, and initiating collaborations and extensions of the research.

Wang received interest from another colleague as well. "Professor Xiaoping Zhang at Wuhan University was one of Max Gunzburger's visiting scholars. His office was next to mine during that one year period. He invited me to visit him as well."

When the sabbatical award was granted, Wang accepted the invitations, visiting two universities – Wuhan University and Huazhong University of Science and Technology – both in east central China, to conduct collaborative research; each visit lasted approximately one month. Wang was asked to collaborate with faculty and staff, and to present lectures to each professor's respective research group.

"At Huazhong University of Science and Technology, I gave a series of four talks to Professor Zhang's research group. I wanted to systematically present my research in mathematical biology, and discuss the application of phase field methods to the study of bio-membranes. Between talks, I met with his students, giving them a forum to ask any follow up questions to deepen and clarify their understanding.

"Professor Zhang shared some of his ideas with me about the proof of the stability of a numerical scheme used in my research. Some of his students will do some further investigation of that problem.

"At Wuhan University, I had a deep discussion with Professor Xiaoping Zhang, in the area of image processing. We discussed Edge Weighted Centroidal Voronoi Tessellations and how the method can be applied in image clustering, and we exchanged ideas about new developments in machine learning. I talked with some students there, and I encouraged them to apply to our department.

"During my trip, Professor Hao Chen at Chongqing Normal University heard about my visit with Professor Chenjian Zhang. Professor Chen strongly encouraged me to visit his research group, and to talk with his students. I was able to visit and give a talk there, and I had some very productive discussions with his students."

Wang's sabbatical benefits the university at multiple levels. For the department, Wang plans to introduce his newly acquired methods and approaches to two graduate courses, Scientific Visualization and Scientific Programming. Concepts and ideas generated through discussions of the most recent developments in image processing techniques (one of Wang's primary research streams) can be used in these courses, and students enrolled in the classes can select projects that apply numerical methods used to solve partial differential equations in individual and group projects. At a broader level, sister departments and the university-at-large can use Wang's collaborations to generate new research in cell numerical simulations, especially in biology, mathematics, medicine, and engineering.

For more, go to
www.hust.edu.cn
www.whu.edu.cn
http://people.sc.fsu.edu/~wwang3/

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effectively lowering the barrier for students to integrate DFT simulations into their research. Working with the outreach programs at FSU, he continues involving middle school and high school students in his research to increase their interests in pursuing STEM careers.

"This NSF award will support my group to continue developing new methods for understanding and predicting electronic properties of material at nanoscale." --- CHEN HUANG

Department of Scientific Computing Chair, Gordon Erlebacher, expressed excitement about Huang's research and accomplishments, saying, "Professor Huang exemplifies what the Department of Scientific Computing stands for: the development of new computational algorithms of societal import. His work skillfully melds Mathematics, Computing and Science to create algorithms that will significantly advance fundamental material science."

Huang earned his Ph.D. in physics from Princeton University in 2011 and was a postdoctoral associate in the Theoretical Division at Los Alamos National Laboratory prior to joining the Department of Scientific Computing in 2014. He is the third recipient of the CAREER Award in the Department of Scientific Computing.

The NSF CAREER Award supports junior faculty in research and career advancement, emphasizing the importance on the early development of academic careers.
For more information on the CAREER Award, go to www.nsf.gov.

For more information on Huang and his group, go to https://sites.google.com/site/huangfsu/home.

For more on the department, go to sc.fsu.edu.

Gunzburger organizes international workshop series

A series of international uncertainty quantification workshops is underway at the Isaac Newton Institute for Mathematical Sciences. The workshops were designed to bring together an international cadre of research scholars and thinkers to learn, exchange ideas, and collaborate over a six-month period. A chief objective of the series is to bring together applied mathematicians and statisticians to study the latest developments in uncertainty quantification, and to exchange approaches to research between the two fields. Five core themes of common interest to statisticians and applied mathematicians provide the focus: (1) surrogate models, (2) multilevel, multi-scale, and multi-fidelity methods, (3) dimension reduction methods, (4) inverse UQ methods and (5) careful and fair comparisons.

"We've been planning this workshop series for about 3½ years or so. Some of the applied math and statistics community have been separate and have separate views on how to quantify uncertainties. One of our goals was to get people from the math and statistics communities together to exchange approaches," said Max Gunzburger, DSC professor and workshop organizer. "We each have some ideas and want to see not who's doing it better, but what approaches or combined approaches work best for which problems."

Uncertainty quantification (UQ) is a method of calculating ambiguity in complex mathematical systems. It is used to study problems such as climate, weather, minor earthquakes, ocean modeling, or can be about designing a car or a car engine. Commercial and industrial vendors are interested in uncertainty as manufacturers need to know how their product will fare given a range of real world conditions. For example, they may want to know whether their product or device will withstand a certain amount of load, or force, and they want to be able to make predictions that correspond to reality as closely as possible.

Max Gunzburger

"When you're solving most computational models, you begin with a computer model, input some data and then get a specific answer based on the model and the inputs. If you have uncertain inputs to the problem – for example, if you're trying to determine whether a hurricane is going to make landfall in a certain area at a certain time -- you begin to deal with probabilities, because you don't know precisely what outcomes to expect, and small changes may mean your calculations are invalid.

Isaac Newton Mathematical Institute

"Applied mathematicians tend to develop very complicated models. When dealing with uncertainty, they try to get a good, accurate description of the problem; this allows them to develop the most accurate model they can. To run one of these very complicated models is very expensive, so they try to get a very accurate description of the uncertainty. On the other hand, statisticians have a lot of probabilistic methods for developing the amount of uncertainty. The workshop series was to get these approaches together for deep collaboration over a period of time."

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Grad student wins prestigious university award

Amirhessam Tahmassebi, a graduate student in the Department of Scientific Computing, recently received an award for exceptional creativity and scholarship. The Graduate Student Research & Creativity Award recognizes the superior scholarship of FSU graduate students. Tahmassebi received the award for outstanding contributions to research and creative endeavors through publications and presentations in the natural and physical sciences, including mathematics and engineering. A doctoral candidate studying medical imaging, Tahmassebi was one of a highly selective group of advanced students recognized for the depth, volume and creativity of his research.

Tahmassebi learned about the award from Professor Anke Meyer-Baese, his mentor and dissertation director. His aptitude for research was apparent early on, when Tahmassebi excelled in one of her courses. “My first interaction with Amir was in my Data Mining course where he went above and beyond in his independent project and proved himself to be an outstanding student. Amir demonstrated the ability to work independently with great creativity and enthusiasm, putting in many long hours. He was usually the first one in the lab in the morning and the last to leave in the evening,” Meyer-Baese said.

For much of his time as a graduate student, Tahmassebi has been involved in a cross-disciplinary approach, combining applied mathematics with machine learning and medicine. His main research is two-fold: (1) incorporating key aspects of neuro-biological networks into intelligent computer-aided diagnosis systems via machine learning algorithms and (2) applying knowledge from CAD systems to cancer research. By observing key biological systems, Tahmassebi has been able to formulate theories, then translate those theories into technical systems.

“One of my primary aspirations is to focus my career on the study of biological processes based on mathematical models and use this high level of abstraction to decode the “language” of cells and to obtain insights into how signals from the environment are processed and how decisions for proliferation or differentiation are regulated,” said Tahmassebi. “I am interested in understanding complex, dynamic systems as seen in nature – such as neural circuits in the brain or gene regulatory networks in cells.”

The depth and originality of Tahmassebi’s research approach and his ability to develop sophisticated computational tools for analysis are the foremost reason he was tapped for the award. Since arriving at Scientific Computing, he has created and implemented highly sophisticated computational models for his research in breast cancer and dementia. Many of these tools can be used in other disciplines with applications to different, unrelated problems.

“In brain research, Amir went beyond the state-of-the-art concept of static graph theory and proposed dynamic graph theory to analyze and predict the temporal behavior of disease. In breast cancer research, he discovered the most important parameters extracted from MRI in the early prediction of the response to neo-adjuvant chemotherapy. For both, he processed multi-parametric imaging techniques and proposed analysis modalities that will lead to a breakthrough in our understanding of both brain and breast disease,” said Meyer-Baese

Amirhessam Tahmassebi

Tahmassebi combines his ability to conceptualize problems from technical, abstract and multidisciplinary prisms and combines it with diligence and prolific writing. He has published nine peer-reviewed papers; in eight, he is first author. He has eleven accepted peer-reviewed papers in the pipeline and will soon be published. His reputation and research is widely admired, and he is working – by invitation – with some of the fields’ most highly regarded scholars, both nationally and internationally.

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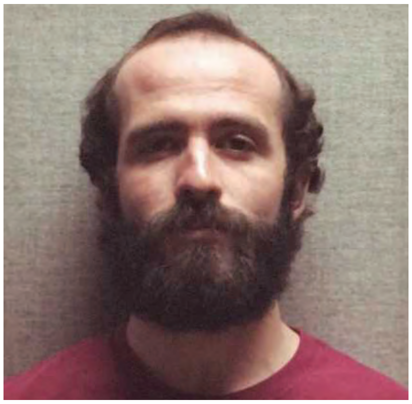
Grad students secure summer internships

This summer, Ezra Brooker plans to participate in a workshop program at Los Alamos National Laboratory (LANL) in Los Alamos, New Mexico. A DSC grad student, Brooker was selected as part of LANL's Computational Physics Student Summer Workshop, sponsored by the Advanced Scientific Computing Division. The workshop has twelve different projects covering topics such as astrophysics, fluid dynamics and molecular dynamics, with 2-3 students assigned to each project.



Grad student Ezra Brooker

Brooker will work with Chris Fryer, a theoretical astrophysicist who made important scientific contributions in the area of core-collapse supernovae, gamma-ray bursts, and supernova remnants. "I will be working with a student from another university as an equal research partner," said Brooker. "Both of us will be mentored by Chris Fryer on his "Stardust" research project. The program is very similar to an REU (Research Experience for Undergraduates) in structure. I will be attending the 10-week computational workshop beginning in June."

Brooker has been working on a loosely related project with his advisor and DSC professor, Tomek Plewa, and hopes to continue this research at the conclusion of the summer workshop with Fryer. "I'll be continuing and expanding on the topic, but I do not know at this time if Chris will be involved after this summer or not. Being admitted to the workshop AND assigned the Stardust project is a textbook example of very fortunate luck!"

Often, workshop participants are required to present their research in a short slide or poster presentation at the conclusion of the program and the project group submits the work for publication or a conference presentation. Brooker will attend the workshop from June 11th to August 17th.

STARDUST PROJECT

Supernovae are the sites of production and dissemination of most of the heavy elements. The distribution of these elements, especially the ratios of different isotopes, can be used to test our understanding of the engine behind these supernovae. Supernova dust grains are one of the leading probes used to study supernova isotopics.

This project will work with multi-dimensional supernova explosion calculations, using statistical methods to compare to dust grain data to constrain the properties of the supernova engine. Depending upon the interest of the students, they will focus on detailed nucleosynthetic yield calculations, dust formation or statistical methods to compare the simulation results to the existing data.

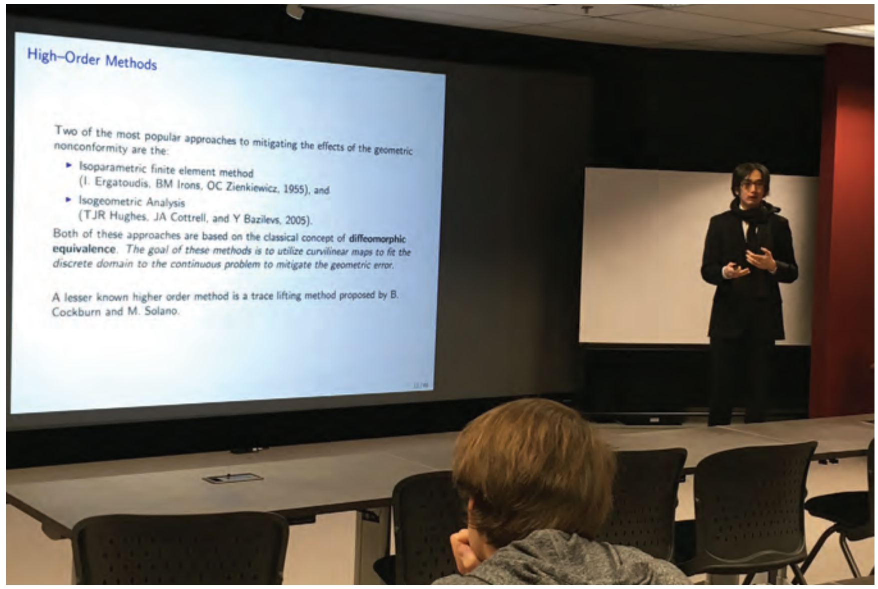
For more on the Computational Physics Student Summer Workshops, go to: http://www.lanl.gov/org/padwp/adx/computational-physics/summer-workshop/index.php.

Celine Nagales explains her research poster at Computational Exposition

Grad student Celine Nagales will intern this summer at the Florida Bureau of Archaeological Research (BAR), located on the property of Mission San Luis. The BAR is responsible for all archaeo-

Cheung studies new methods using polynomial extensions

James Cheung, a student of Professor Max Gunzburger, has completed the requirements for the Ph.D. in computational science. Most recently, Cheung was a Graduate Student Research Assistant for the department. During his years as a student, he interned at Oak Ridge National Laboratory in Tennessee, and Sandia National Laboratories in Albuquerque, New Mexico. At Oak Ridge, Cheung worked on the development and analysis of a two-level sparse grid collocation method for reducing the cost of determining the expectation of hyperbolic stochastic PDE by using asymptotic series model reduction. At Sandia, Cheung worked on the development and implementation of a Schwarz alternating approach for the nonlocal-to-local coupling of the classical density functional theory equations to the Poisson-Nernst-Planck equations on HPC clusters.



James Cheung presenting his research

Cheung's dissertation, Overcoming geometric limitations in the finite element method by means of polynomial extension, presents a new approach for approximating the solution of second order PDE and interface problems. Using the finite element method, Cheung used polynomial extensions to enforce that a suitably constructed extension of the numerical solution matches the boundary condition given by the continuous problem. This approach is simple to implement and is optimally convergent with respect to the best approximation results given by interpolation.

"As a student of the Department of Scientific Computing, I felt that there were many opportunities for academic, professional, and personal growth," said Cheung. "The interaction with students and faculty here have opened my mind to the many different facets of science – something that is seldom found in other academic departments." James will work as a postdoctoral research assistant in Professor John Burns' group in the Interdisciplinary Center for Applied Mathematics at Virginia Tech. His research will focus on numerical solution methods for Riccati equations in relation to optimal control theory.

For more, go to sc.fsu.edu.

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logical materials recovered on state lands and state waterways. As part of her project, Nagales will be using photogrammetry to render 3D models of the artifacts of the Maple Leaf, a shipwreck which sank off the St. Johns River near Jacksonville during the latter part of the Civil War. The ship was retrieved from the St. Johns in 1984; because the ship was encased in mud, its contents were preserved. The collection of artifacts from the Maple Leaf shipwreck was originally cataloged in the 1990s.

"The Maple Leaf collection includes an officer's sword, pieces of a violin, china sets – it's a large project with many pieces," Nagales said. " I'll be scanning the pieces into a database and experimenting with different scanning methodologies to include a laser scanner, from the Morphometrics Lab, and photogrammetry. "

Once these objects are completely rendered in 3D, these models will be shared with the public online. The BAR is currently exploring means of sharing the collection online and has developed a website to showcase collections that represent the history of Florida here: http://floridahistoryin3d.com/.

Nagales will begin working with the BAR in early summer with Dr. Steve Karacic and Dr. Kathryn O'Donnell Miyar.

For more, visit
http://www.mapleleafshipwreck.com
http://morphlab.sc.fsu.edu/

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The department's mission is to be the focal point of science and computation at Florida State University. Gordon Erlebacher is Chair of the Department of Scientific Computing. He can be reached at 850.644.7024. Newsletters are issued three times each year. Subscriptions and single copies are available by calling 850.644.0196. This publication is available in an alternative format on request.

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The Graduate Student Research & Creativity Award is made annually in the spring term through the Graduate School and the Office of Research at FSU. Recipients must show evidence of outstanding scholarship, creative productivity, and national visibility in research. Tahmassebi received one of only six awards university-wide.

For more, go to:
gradschool.fsu.edu
amirhessam.com

For related story, go to sc.fsu.edu
http://news.fsu.edu/news/2018/04/18/fsu-honors-graduate-students-for-teaching-scholarship-and-service/.

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Gunzburger, along with Peter Challenor (University of Exeter), Catherine Powell (University of Manchester), and Henry Wynn (London School of Economics) worked with the Newton Institute to develop this thematic workshop series, and Gunzburger gave lectures earlier in the series and will present another workshop at the concluding session in June.

Scientists from North America, Europe and Asia were invited to attend with some attendants choosing to stay for a week, others for much longer. The workshop series is sponsored by the government of the UK, the Simons Foundation, Rothschild & Company, The London Mathematical Society, and Clay Mathematics Institute.

You can watch the workshops live online at http://www.newton.ac.uk/events/streaming.

You can see a presentation Gunzburger made earlier in this series by going to http://www.newton.ac.uk/seminar/20180109100011001.

You can find out more about the department at sc.fsu.edu.

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