Department of Scientific Computing

Spring 2014

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SC's Developing Scholar, Ming Ye

Associate professor and computational hydrologist Ming Ye is a 2014 recipient of the university's Developing Scholar Award, an honor bestowed on mid-career, associate professor level faculty to support their research programs. Ye was selected as a Developing Scholar by the university's Council on Research & Creativity, the Vice President for Research, and the President. The Developing Scholar Award is based on evidence of a clearly established program of research and creativity lasting over a number of years – a record of superior research and creativity that has garnered external recognition. The award was created to identify FSU's future academic leaders at an early mid-point in their careers and to promote faculty research and creativity during the academic year following the award. Ye was nominated by SC Professor Michael Navon, with enthusiastic endorsements from SC Chair Max Gunzburger, Arts and Sciences Dean Sam Huckaba, and wholehearted support from external collaborators and scholars.

The basis of Ye's nomination and subsequent award stem from an extensive career of innovative and cited research in top-level, peer reviewed journals; prestigious external awards such as the Department of Energy Early Career Award; myriad, significant grants as the sole principal investigator; accomplished student mentoring and course development activities; and collaborative relationships that span the globe. When talking about the many aspects of his work, Ye is eager and animated. He has ongoing research on nitrogen contamination in St. Lucie, Indian River and Martin counties. There is also a major project with the Department of Energy to study how to quantify predictive uncertainty in groundwater reactive transport modeling using computationally efficient methods. Right now, one primary focus of his research is the study of sinkholes, one of Florida's critical environmental issues.

"Last year, we got a CRC project to study sinkholes. It's multidisciplinary support with Xiaoming Wang, professor and chair in Mathematics. Sinkholes are everywhere. If you went up in an airplane to get a high-level perspective, you would see these circles and ponds on the ground. These are sinkhole lakes. Down south and in the central

Ye's lab performing an experiment.

portion of the state it's much worse than it is here, but we do have them here in the northern part of Florida. For instance, we have sinkholes at FSU Innovation Park and Leon Sinks Geological Area on Crawfordville Road just fifteen minutes away from the campus. In 2002, Lake Jackson just disappeared suddenly into two sinkholes – Porter Sink and Lime Sink."

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The study of sinkholes is important for the entire US, and for countries abroad. Data from the United States Geological Survey (USGS) on sinkholes shows the frequency and extent of their occurrence. Even Ye, a geology scholar, finds the data surprising. "There are some statistics from USGS that have some really astonishing data. Twenty-five percent of US geology is covered by KARST topography, and nearly twenty percent of US terrain is subjected to sinkhole events. It's just incredible to think that sinkholes can occur anywhere, and with Tampa and Orlando, we're here in the nation's capital of sinkholes."

Ye and his students and postdocs are doing a sinkhole study at GFDI, the Geophysical Fluid Dynamics Institute. The sandbox is ready, and they are preparing a demonstration experiment. He also plans to continue his work on sinkholes by visiting one of his collaborators in Reston, Virginia, at the USGS. "I have a collaborator there who's going to take me out into the field, show me some sinkholes there, and talk about the research they're doing on them. I think we'll have some mutual research interests and the possibility of future joint projects."

In addition to Florida and Virginia, there has been both national and international interest in Ye's work. NOVA, one of PBS's award-winning science-based programs, is planning to do a program on sinkholes. As part of the program, they came down to interview people from the geological survey. Part of Ye's work – the model he is using – was demonstrated and used in the experiment. Internationally, Ye continues his work in China and Europe with visiting scholars, students, and governmental officials.

Ye at the Skyline Caverns sinkhole in Virginia

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>
> MING YE

Recipients of the Developing Scholar Award receive a one-time award of $10,000 to be used in their research program. With these additional funds, Ye intends to continue experimental study of sinkhole development and collapse. "I want to use the money for student support on the project, and to travel to Europe and China to collaborate with colleagues. China, especially, has some of the same issues we have here with the environment, and to be able to continue to work with them on these issues is critically important and mutually beneficial."

To see video footage of a sinkhole experiment done by the Ye lab, go to http://youtu.be/275oWFUzgOg.
To see Lake Jackson as it drains into a sinkhole, go to www.youtube.com/watch?v=NpbczFIKH8I.
For more information on sinkholes, go to http://water.usgs.gov/edu/sinkholes.html.
For more on Ye, go to sc.fsu.edu.

SC shines at SIAM

Scientific Computing was well represented at SIAM meetings in March and April. Students, researchers and faculty presented at all meetings. SC department chair Max Gunzburger was one of the organizers for the SIAM Conference on Uncertainty Quantification held in Savannah, Georgia, March 31-April 3.

This meeting brought together experts and novices to discuss ideas, collaborate, network, and present research findings. Uncertainty quantification is a broad field, which includes the characterization and estimation of "natural" errors and control of computational error, the modeling and analysis of data which is only partially known, and the development of techniques that can produce reliable results despite the presence of errors, uncertainties, and incomplete data.

Gunzburger gave a talk titled, A Generalized Stochastic Collocation Approach to Constrained Optimization for Random Data Identification Problems. Professor Ming Ye spoke on A Bayesian Framework for Uncertainty Quantification with Application to Groundwater Reactive Transport Modeling.

Other talks were given by graduate student Tim Handy, by postdocs Aretha Teckentrup and Hans-Werner van Wyk, and by research programmer John Burkardt. Two graduate students, Michael Schneier and Wenju Zhao, also attended the meeting.

For more information on SIAM, go to siam.org.
To see pictures from one of the SIAM meetings, go to our Facebook page.
https://www.facebook.com/FSUSciComp.

Attending SIAM in Savannah was a valuable opportunity to network for graduate student Mike Schneier. In addition to attending the presentations and workshops, Schneier secured an internship position for the summer. Schneier will spend the summer at Oak Ridge National Laboratory working with Clayton Webster, who is on the Predictive Mathematics Team.

"I met Clayton in Savannah at SIAM. We talked there about the research he was doing, and he asked whether I'd be interested in coming to Oak Ridge this summer to do an internship. I accepted on the spot!"

Schneier will work on a reduced order modeling problem with applications to stochastic partial differential equations which are used to model physical phenomena and processes. He will be in Tennessee from June 9 – August 15th.

Below, clockwise from left: Rui Gu presenting his research, Danial Smith discussing research findings, John Burkardt gearing up for a session, & Hans-Werner van Wyk (left) putting up a poster.

Learn to intern at Livermore

When SC doctoral student Ryan Learn applied for internship positions in February, he was absolutely positive about one thing. "I had written off getting this internship. I applied for four different positions, and this is the one I thought – There's no chance. This one would be the coolest, but there's no chance." Ten days later, Learn had the summer internship he wanted.

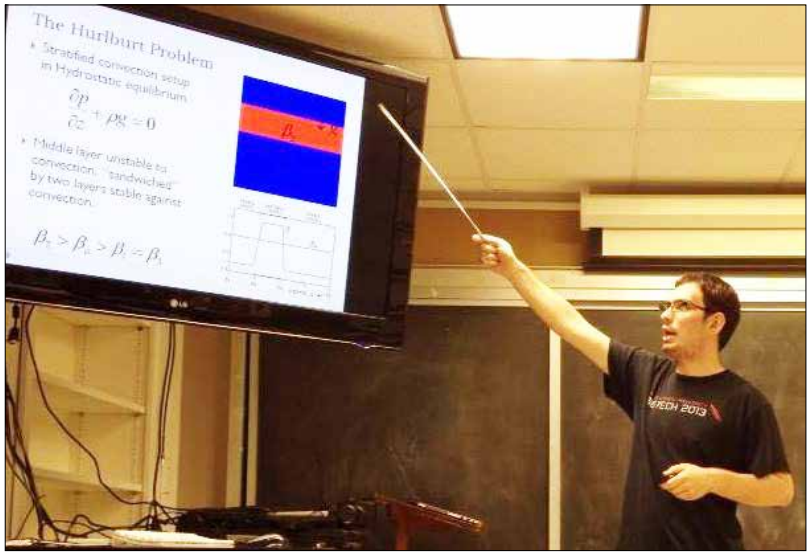
Learn will spend this summer at the National Ignition Facility at Lawrence Livermore National Laboratory. The highest energy laser system in the world, the NIF facility uses 192 laser beams to create temperatures and pressures similar to those that exist only inside nuclear weapons and in the cores of stars and giant planets. As the premier high energy laser and photon facility, the laser beams at NIF are capable of delivering 100 times the energy of any previous laser system.

"I'm going to be doing calibration studies on beam propagation. In this type of research, it's important to understand the lasers and their capabilities. So if you have 192 lasers pointing at a little tiny spot of deuterium, then you increase the density and temperature, you sort of compress it. If you get it hot enough and dense enough, you make the deuterium fuse into helium. That's the fuel source of the sun, so the lasers sort of recreate the conditions of the sun on a much smaller scale."

Learn applied for the position at NIF on a Tuesday. That Friday, he got a phone call from Eyal Feigenbaum, an electrical engineer and Livermore research scientist who uses the NIF lasers to simulate the density and temperature of nuclear objects and to study how nuclear weapons age. As the interview with Feigenbaum concluded, Learn had a good feeling about the position. "I talked to Dr. Feigenbaum by phone that Friday at around 6pm. When he talked about what he wanted to do for the summer, so much of it was familiar. The code I'm working on here simulates plasma hydrodynamics. Feigenbaum's code simulates the lasers that are going toward the deuterium. When you have all those lasers, you want to be able to control how they work, and simulate how they work. So if you want to have any understanding of how things will go, you need to know how the lasers interact with the fuel and the atmosphere. At the end of the interview, he said it sounded like I was qualified for the position, and they'd be in touch. That made me feel confident and encouraged." A short time later, Feigenbaum offered Learn the internship.

The work of the internship has two distinct phases. First, Learn will focus on calibration studies; following that, he'll test boundary conditions. "I'll be working on these computer codes, essentially calibration studies on their beam propagation. That'll be the first part of the summer. If I get through with that, I'll be working on new boundary conditions for the code, which is something I've been working on here, so I've already got experience doing that. I've done all sorts of boundary conditions on our code."

Learn is one of two students selected to intern at NIF; approximately 250 students intern at Livermore during the summer. "NIF is the be all and end all of high energy lasers in the world. And Tomek is a principal investigator on an experiment there. So it's kind of like a particle physicist going to CERN. It's really cool. I am very, very satisfied." Learn plans to leave for California on May 19th.



Learn giving a presentation as part of the 2013 Geophysical Fluid Dynamics Institute Seminar series.

Graduation, next steps for grad students

Michelle Perry accepted a postdoc position starting in May at the National Superconducting Cyclotron Laboratory (NSCL) at Michigan State University. Perry will be a Research Associate in the Nuclear Physics group where she will work to improve functionality in the LISE++ software. The LISE++ software is used in various labs across the world. It simulates nuclear physics experiments, allowing users to optimize spectrometer parameters for their experiments and estimate reaction products.

NSCL is a world-leading laboratory for rare isotope research and nuclear science education. With support from the U.S. National Science Foundation, the laboratory operates as a national user facility that serves more than 700 researchers from 100 institutions in 35 countries.

Michelle Perry greeting attendees before her dissertation defense.

"The postdoc I accepted was my number one choice out of all the positions I applied for. It also happens to be the only one I didn't apply for. The lab contacted me about the postdoc. I had interviewed there for a different position so they had my CV. They thought I may be a good fit and scheduled me for an interview. They hadn't posted the position yet which is why I hadn't applied. I applied for many other positions of all types. I really wanted a postdoc associated with experimental physics, so I cancelled a couple future interviews for other positions when I received this offer."

Perry graduated with the Ph.D. in Computational Science in May, and she credits Professors Anke Meyer-Baese and Harrison Prosper with sparking her enthusiasm for her research. "The final project in Dr. Meyer-Baese's Data Mining course set me on the path to my research topic. In doing the project, I learned that neural networks were used in experimental high energy physics. I was so interested in it, I met with people using these methods in the Physics department, which led to a DIS project. In doing the DIS project, I decided that this was something I really wanted to do my dissertation work on, and was happy when Dr. Meyer-Baese and Dr. Prosper agreed to be co-advisors on my project.

"I found the flexibility in research areas helpful for my graduate work. I was able to seek and find something that I truly found exciting."

Perry would like to continue doing research related to experimental physics in any way possible, whether through a staff position or as a professor. The position at NCSL is a two-year position.

Perry is one of four grad students who completed degrees in the department this Spring. Others include:

* Daniel Fenn, who completed the requirements for the Master of Computational Science. He is returning to Scientific Computing to pursue the Ph.D.

* Timothy Handy, who completed his Ph.D. Tim accepted a one year postdoc with his professor, Tomek Plewa.

* Kushal Venkatesh, who completed his masters degree. Kushal accepted a position at Nielsen in Tampa, FL. Nielsen studies which television shows people watch and other consumer behaviors to provide trends and habits worldwide.

For more on NSCL, go to http://www.nscl.msu.edu/.
To see Perry defending her dissertation, go to www.facebook.com/FSUSciComp/.

New grad students, post doc

Maliheh Shaban Tameh

MALIHEH SHABAN TAMEH, a doctoral student from Tehran, Iran, received her masters in Quantum Field Theory & Fundamental Particles Physics in 2009 from Shahid Beheshti University. Tameh graduated from Tarbiat Moallem (Kharazmi) University with a Bachelor of Science in Solid State Physics in 2004.

An experienced researcher, Tameh uses a variety of methods to solve differential equations, including meshless, finite element, homotopy analysis, shooting, and Discontinuous Galerkin. As a masters student and research assistant, she studied radial basis functions, simulation of physical systems with space and time dependence, and the development of numerical methods for solving PDEs, ODEs, FDEs and nonlinear systems. She has published in many journals, including the International Journal of Computer Mathematics, Applied Mathematics and Computation and Mathematical Methods in the Applied Sciences.

When she is away from her research, Tameh quotes poetry, enjoys reading novels, plays volleyball, and cooks her native Persian food. Tameh's professor is Max Gunzburger.

Cameron Berkley

No stranger to Scientific Computing, CAMERON BERKLEY entered the graduate program after completing his undergraduate degree in computational science. Berkley is from Jacksonville Beach, Florida, and started his undergrad studies at Florida State College at Jacksonville. He transferred to FSU in his sophomore year as an applied math and computer science major.

After taking Introduction to Scientific Computing with Dr. Dennis Slice, Berkley switched majors to computational science and joined the geometric morphometrics lab. In the lab, he worked with the US Army Natick Soldier RD&E Center studying variation in cranial shape for helmet research, and developed a novel camera calibration method for his undergraduate thesis project.

In his leisure time, Berkley likes to listen to music—especially blues rock and psychedelic rock—and builds and flies high-performance radio controlled helicopters.

Anahid Ehtemami

ANAHID EHTEMAMI is from Tehran, Iran, and discovered her love of programming at the age of 18 when she moved to Malaysia. In March 2013, she received the Bachelor of Science in software engineering from Asia Pacific University of Technology in Kuala Lampur. For her undergraduate project, she combined her love of music with her software engineering skills and developed an online music theory training system for children using ASP.NET. She also programs in C, Visual Basic, Java, HTML, and AJAX. After graduation, she spent a few months in Iran with her family while studying and researching different areas that she could choose for her graduate studies. She started her graduate studies in Spring 2014; her main areas of interest are bioinformatics, phylogenetics and evolutionary biology.

She loves playing the violin, mathematics, algorithms, and design. Ehtemami is pursuing her Master of Computational Science.

Michael Schneier

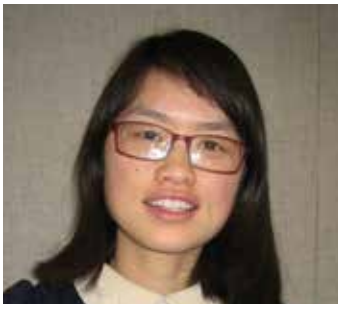
MICHAEL SCHNEIER is a Masters student from Queens, the eastern-most borough of New York City. He received his undergraduate degree in mathematics from the University of Pittsburgh in April 2013. In addition to programming in Fortran, Schneier taught pre-calculus while still an undergrad.

In his free time, Schneier enjoys hiking and playing Frisbee. Currently, he is working on high dimensional interpolation research with Max Gunzburger, and is teaching spreadsheets as a Teaching Assistant at the Program for Interdisciplinary Computing. Schneier will be spending the summer as an intern at Oak Ridge National Laboratory. See related story, page 3.

Lukas Bystricky

LUKAS BYSTRICKY of Thunder Bay, Canada received his undergraduate degree from the University of British Columbia in mathematics in May 2012. He was a co-op student at Automotive Fuel Cell Corporation, a joint Daimler/Ford venture and global leader in fuel cell stack development. In that position, he ran multi-physics simulations for customers in MATLAB and COMSOL, calculated temperature distribution along width/length of fuel cells, investigated effects of operating conditions on water distribution in side fuel cells, ran optimization projects, and validated models with experimental data. During the year following graduation, Bystricky was the lead programmer at Mitomics, Inc, a biotech research company investigating commercial applications of mitochondrial DNA for cancers.

Bystricky is a member of the Northwestern Ontario Civilian Air Search and Rescue, and in his spare time, he plays squash with the FSU squash league, plays guitar and piano, reads 20th century technological history, and enjoys listening to music. He plans to work with Janet Peterson and Sachin Shanbhag modeling the orientation of carbon nanotubes in fluid.



Yan Zhu

YAN ZHU, a new post doctoral associate, is from Anhui Province in central China. In 2007, she graduated with a degree in engineering from Wuhan University in Hubei Province, one of the most beautiful campuses in China. As an undergrad, Zhu had internships which provided many opportunities to travel to different parts of the country.

Zhu began the combined masters-doctoral program at Wuhan U. in 2009 majoring in groundwater resources and environment. As a student, she completed detailed research programming models to calculate water flow and solute transport in the subsurface system. During her Ph.D. studies, Zhu spent two years in Canada at the University of Waterloo doing water flow simulations in coupled surface and subsurface systems. Zhu graduated with the Ph.D. in engineering in 2013.

Zhu is spending this year as a postdoc with Ming Ye, adding an ammonium module to ArcNet, a model for simulating groundwater flow and nutrient transport.

Zhu has been happily married for three years and enjoys reading, jogging and playing badminton.

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The department's mission is to be the focal point of science and computation at Florida State University. Max Gunzburger is the 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.

Outstanding research presented at Xposition

The highlight of the Spring semester, the 2014 Annual Xposition included innovative research on a broad array of topics. You can find more pictures of the students' posters at our Facebook page, www.facebook.com/FSUSciComp.