Department of Scientific Computing

Fall 2016

Meyer-Baese receives Fulbright Award

Scientific Computing professor Anke Meyer-Baese has been awarded a Fulbright Research Scholarship, a prestigious, highly competitive merit-based award for scholars and scientists created by treaty in 1948. The Fulbright Commission fosters mutual cultural understanding through educational exchange between nations.

Meyer-Baese will do research in Alsace, France based at the ICube Laboratory at the University of Strasbourg. Created in 2013, the ICube Laboratory is a state of the art biomedical engineering and imaging research facility centered on medical and surgical imaging and robotics, the environment and sustainable development, scientific computing, imaging physics and systems, and material engineering for energy and environmental applications.

Meyer-Baese will spend six months in France applying advanced dynamic graph networks to dementia research.

"Dementia with Lewy bodies (DLB) is the second most common dementia after Alzheimer's disease (AD). The overlapping clinical symptoms of DLB and Alzheimer's disease make differentiation between these two neurodegenerative diseases difficult. Neuroimaging methods have provided important information on differences in specific structures between AD and DLB patients that can be used to enhance diagnostic accuracy.

"The research for this Fulbright award will provide a fast and accurate computational diagnosis support based on neuroimaging techniques for the clinical neuroscientist to assist him in identifying DLB patients at an early stage and evaluating their disease evolution," said Meyer-Baese.

Professor Meyer-Baese teaches courses in Data Mining and Computational Methods for Discrete Problems. She is the author of over 200 journal articles, many conference publications and three books.

For more on the ICube Laboratory, go to https://icube.unistra.fr/en.
For more on the Fulbright Scholar Program, go to http://www.cies.org/.
For more on Professor Meyer-Baese, go to https://people.sc.fsu.edu/~ameyerbaese/research.html.

Professor Anke Meyer-Baese at right.

Professor receives NSF Grant

Ye award to integrate data-worth analysis into framework of multimodel analysis by using uranium contamination at Naturita Site [Colorado], and nitrogen contamination site at Indian River County [Florida].

Professor Ming Ye has been awarded a three-year $450,000 grant by the National Science Foundation to study new models for groundwater remediation. Groundwater contaminant remediation involves removing subsurface contaminants so they do not pose unacceptable future risks to humans and the environment.

"This grant will help answer the question of where and when to collect data, an issue important not only to environmental modeling but also to almost all fields involving numerical simulations," said Ye. "We will develop mathematically rigorous methods, and evaluate them with real-world data. We plan to apply the methods to the nitrogen pollution problem in Florida. This will leverage my project funded by the Florida Department of Environmental Protection, in which field data have been collected, but more are needed to understand the fundamental reasons of eutrophication that is threatening Florida waters."

The research will focus on groundwater contaminant remediation design under model uncertainty by using a multi-model-based data-worth analysis. In this approach, multiple models are used to identify and guide collection of the most valuable data for model evaluation, improvement, and reconstruction. Because of the synthesis between models, remediation designs and data, the proposed analysis will provide a transformative platform for scientists, engineers, and decision-makers to systematically investigate all components involved in groundwater remediation. The project will also provide an opportunity for interdisciplinary training of undergraduate and graduate students in the areas of hydrology, computational science, and civil engineering. The project will engage high school teachers and students in summer schools to gain laboratory and computational experience for understanding the concepts of groundwater contaminant transport and remediation.

The research has two objectives: to reformulate data-worth analysis for groundwater remediation with consideration of model uncertainty, and to break computational barriers between models and model analysis needed for remediation design. Professor Ye will serve as Principal Investigator for the grant, and will work on the project from August 1, 2016 through July 31, 2019. He will collaborate with Roseanna Neupauer and Joseph Kasprzyk at the University of Colorado at Boulder.

For more, go to http://www.nsf.gov
https://people.sc.fsu.edu/~mye/

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New course on Computational Thinking

John Burkardt preparing to give a course lecture.

Computational Thinking - ISC 1057

It is clear that computers can almost imitate human-like intelligence. The evidence of this is everywhere around us: movie, book and music recommendation systems; programs that allow us to experiment on models of the earth; medical imaging software that can detect tumors that humans can't see. This course asks how computers have gained this ability. The answer includes our detecting patterns in nature, but also patterns in the very way we think. This course will present popular computational methods shaping our lives, and try to explain the ideas that make them work. Students will practice logical thinking by working with versions of these computational methods that affect society and science. Knowledge of a computer programming language is not required nor will it be taught. Grades are based on class participation, homework and group projects.

A new course is available through the department that fulfills the university's quantitative and logical thinking requirement for all undergraduate students. The requirement is designed to help students critically analyze quantitative and logical claims by using a variety of appropriate methods to represent and solve real world problems.

Computational Thinking considers the nature of problems and restructures them computationally - logically, algorithmically and recursively - so that computers can assist humans in solving those problems. During the course, students think about what types of problems are amenable to being solved on the computer. Then the course explores the

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Ph.D. grad uses data science to advance health

Arsia Takeh talks about his time since leaving the department and his new position as Head of Analytics and Data Science at Precision Wellness

When I graduated with the Ph.D. in Computational Science, I got an offer from Advanced Cooling Technologies, Inc. (ACT) as a Research and Development Engineer I at Defense and Aerospace Division, Advanced Computational Modeling Group. I was notified about this position through an SC affiliate and former postdoc - Dr. Srujan Rokkam - who was already working there. ACT is a premier thermal management solution company located in Lancaster, PA -- 45 minutes outside of Philadelphia. I primarily engaged to be involved in a laser modeling project. The goal of that project was to develop physics-based models to predict the behavior of mid-IR Bismide doped lasers. This involved a great deal of understanding the physics of the problem while simultaneously implementing a stable mathematical model which could optimize computational resources.

Besides the project I worked on, I wrote proposals for two other projects and was indirectly involved in writing three additional proposals. The proposals I wrote were to introduce statistical modeling -- particularly Bayesian inference -- into the field. This was unprecedented.

Doing all these tasks required a wide range of skills. The skills I learned in my years at SC including statistics, computational modeling, mathematical modeling, optimization, computational materials, and programming were very valuable, as were those I learned during my tenure at ACT. The skills I learned at ACT were very diverse and depended on the type of project I was working on. The great thing about ACT is its collaborative environment; they tried to maximize collaboration through all projects within the group and even the company. I got promoted to R&D Engineer II within 4 months of starting my work at ACT; this was the fastest promotion period in the company. After 10 months of working at ACT, I had to leave the company and move to California for family reasons; this started the next chapter of my professional career.

My new position is at Precision Wellness, a healthcare start up located in Redwood City, CA. I'm head of analytics and responsible for designing the analytics engine of the product. The analytics engine is the core of the product, and we're defining our IP around this engine.

We are in the precision medicine realm, which aims to offer personalized health recommendations for every individual based on their genetics, family history, and other specific characteristics.

Our customers, though, are not individuals; what we analyze is insurance holder populations. We categorize these populations according to their relevant cohort based on their risk level. Insurance holders can fall into low risk or high risk categories, those who already have the disease or have pre-disease conditions. We approach each of these cohorts uniquely, and try to manage their risks accordingly. It's very important to identify high risk customers so there can be early interventions. By doing so, we can reduce costs, increase the population health, and at the same time increase profit by not spending on managing catastrophic events.

Start up companies are a totally different world; someone has an idea, then thinks how to expand on that idea, how to evaluate new ideas, and how to validate these ideas for the market. Due to the size and nature of the project, we had to have more data scientists on board, so there are data scientists and data engineers who are working under my supervision; I have to manage staff, assign tasks to them, and monitor their daily progress.

There is an extensive collaboration between my team, our clinical team, and our advisors at Stanford University. Stanford's math department, medical school and Genome Technology Center collaborate with us. We also work with financial advisors to validate our approach on the financial side of the problem.

I have daily meetings with our Chief Medical Officer to make sure our clinical assumptions are valid; he guides us on the different treatment scenarios. These recommendations are based on more than 1500 research papers that are analyzed and summarized by the clinical team.

Because our CMO is a cardiologist, the first version of our product will address cardiovascular diseases, the number one killer in the world. By 2030, 40.3% of the U.S. population will have some type of cardiovascular disease. By that time, annual direct medical costs associated with cardiovascular diseases are projected to rise to more than $818 billion, while lost productivity costs could exceed $275 billion.

It is a very interesting story how I found out about this company. Prior to joining Precision Wellness, I was collaborating with an IBM business partner. They were offering predictive analytics solutions for all businesses. I worked there for about a year and accomplished a lot while I was there.

During that time, I participated in a competition held by IBM and The Weather Company, and my team did well! We ranked second among all participants. For our project, we developed an app for businesses and consumers which was able to provide real-time insights for retailers and give them predictive suggestions about customer load based on many factors including weather predictions, socio-economics and demographics.

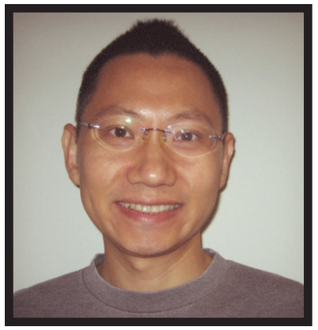
I met the owners and investors of my new company in a meeting, and they discussed their project and asked if I might be interested. I really liked the impact and mission of the project so I considered it seriously, especially since my previous employer decided to change their business model to focus only on predictive solutions for IBM. That's always the risk of working with start-ups; they face financial problems or new opportunities and they change their route. Because there was a stable and growing market, there could have been great financial benefits for me if I stayed, but I want to do something meaningful and learn new things.

If I were to give advice to the students who are working toward their degrees, I only can say try to work and learn as much as you can. Today's world is interdisciplinary and multi-disciplinary and you have to have diverse sets of skills to be able to solve a problem. Another important thing that helped me a lot is being able to complete tasks on my own and at the same time be an effective team player when necessary. You have to be flexible to include any opinion when it's valid; sometimes it's difficult to do so because that means disruption in your process, but you have to compromise to accomplish better results and have a better product. I would also suggest that you look into industry, see the trends, and familiarize yourself with the corresponding job market. It's very important to match your skills and interests with the needs of society and your relevant industry. That would help in any job search and make it easier.

Arsia Takeh pictured with his bride, Hoda Mirafzal, July 2016.

New to Scientific Computing

Seth Boren



Yu-Chieh Chi

Konstantin Pieper

Seth Boren studied Biology and Anthropology at Hendrix College, a private liberal arts college in Conway, Arkansas, located about thirty miles from the state capital of Little Rock. After graduating from Hendrix, his archaeological interests took him northwest to the University of Arkansas-Fayetteville where he completed the Master of Arts degree in Anthropology.

Largely due to the capabilities 3D modeling has for facilitating data collection, Boren's interest in archaeology has branched into morphometrics. He works with Dennis Slice in his morphometrics laboratory where he is learning how to make 3D models of bones and artifacts in order to preserve archaeological data. Boren plays board games and makes ink sketches of animals in his leisure time. Here's a sample of his work.

SC doctoral student **Yu-Chieh Chi** is originally from Kaohsiung, Taiwan, a municipality located in the south west on the banks of the Taiwan Strait. Kaohsiung City is the largest geographical municipality and the second most populated city in Taiwan. Chi studied computers and physics at Southern Illinois University, where he obtained his bachelor's and master's degrees.

With research interests in parallel computing and computational quantum materials science, Chi plans to work with Chen Huang in pursing his Ph.D.

In his free time, Chi enjoys cooking, traveling, hiking, music and movies with his wife, Michelle. He also enjoys spending time with people from many countries and cultures so as to learn about the world.

SC postdoctoral associate **Konstantin Pieper** received his doctoral degree in mathematics from Technische Universität München, located in the largest city in the German state of Bavaria. Pieper published several papers on optimal control with his advisor, Boris Vexler, during his studies, and took finite element discretization and efficient numerical solution of elliptic and parabolic sparse control problems as a dissertation topic. Pieper graduated in 2015.

Since arriving at Scientific Computing, Pieper has been involved in a research collaboration with mathematics Professor Lili Ju at the University of South Carolina along with Max Gunzburger, Lindley Graham, Kenneth Sockwell, and Huanhuan Wang. The group met at USC in November to discuss research and scholarly ideas.

New grad student **David Robinson** grew up in a small dairy and farming community in Merced County, California called Hilmar. He attended San Francisco State University where he earned a bachelor's degree in Astrophysics, and did a senior project that consisted of a parallelized n-body simulation to explore whether heating from collisions was a contributing factor in planetesimal formation.

With the help of Bryan Quaife and Ken Speer from the Geophysical Fluid Dynamics Institute, he is working to develop a fire dynamics model. For fun, Robinson likes to play games on his computer, and he enjoys playing billiards and outdoor activities such as hiking and golf.

Marjan Sadeghi is from Tehran, Iran's capital city. She graduated from K. N. Toosi University of Technology, in 2010 and 2012 with bachelor's and master's degrees in applied mathematics. Toosi University is considered one of the most prestigious government-sponsored institutions of higher education in the nation.

Sadeghi taught mathematics courses during her time as a student, and was a math and chemistry teacher at Razieh High School in Tehran after completing her masters studies. Her research interests lie in numerical analysis, computational mathematics, integral equations, probability, special functions, optimization, operations research and data mining.

While at university, Sadeghi used her service on the Students' Mathematics Council to collaborate in running programming workshops for undergraduate mathematics students. These workshops in C, C++, C# and FORTRAN were to improve students' programming skills. In addition, she was executive editor of Mokhtasat Magazine, and was student representative of the Iranian Society of Cryptography.

Masters student **Kyle Shaw** grew up in Idaho, then spent two years in South Africa on a mission for his church. After returning to the states, he attended Brigham Young University – Idaho in Rexburg, located in the eastern part of the state. While at BYU-Idaho, he studied mathematics, graduating with a degree in math and a minor in computer science. Currently Shaw works with Peter Beerli and is doing research in population genetics. Shaw adapts easily to the activities his environment and the climate permit.

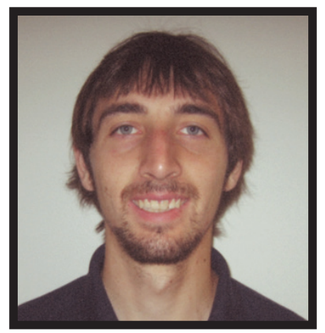
While in Idaho, he hiked, played soccer and ran cross country. Now that he is in Florida, he looks forward to getting scuba gear and learning to dive. He lives with his wife, Miriam.

Xueming Zheng chose Beijing Forestry University – an environmentally friendly university affiliated with China's State Forestry Administration – to pursue her undergraduate degree. She received the bachelor of science in mathematics and applied mathematics in 2016. While an undergrad, she did research on outliers screening and high dimensional data analysis. Zheng plans to work with Ming Ye while pursuing her master of science/doctor of philosophy degree in computational science. Her research will focus on sensitivity analysis for identifying important processes and parameters under model uncertainty.

Zheng enjoys many hobbies, including painting, cooking, swimming, and hiking. She also plays Guzheng, a Chinese musical instrument that has sixteen strings and movable bridges that is played with picks worn on either hand.

David Robinson

Marjan Sadeghi



Kyle Shaw

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Computational Thinking, continued from page 3

A Computational Thinking student responds to a set of survey questions by using her smartphone.

logic behind existing computational approaches for problems as diverse as climate modeling, medical image analysis, genetic descent, modeling galaxies, page rank, and apportionment of voting districts. For each computational approach, students investigate a simplified version of the code's strategy to gain hands on experience.

The course was developed by Janet Peterson and John Burkardt; they currently serve as joint faculty for the course. Students explore ideas that make computing complicated tasks possible such as machine learning, discretization and the discovery of patterns in data.

The class participation portion of the final grade is assessed through the use of clicker technology. Students use their cell phones to respond to questions and surveys; this assessment tool helps record attendance (half the course participation grade) and gives Burkardt and Peterson early and consistent insight into whether and what students are learning and retaining during the course lectures.

To see more about Computational Thinking, including when it is offered in the approaching semester, go to https://www.sc.fsu.edu/courses.
The Department of Scientific Computing is online; check us out on Facebook or send us a Tweet.

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