Department of Scientific Computing
Summer 2012

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Ye receives Department of Energy Early Career Award

SC Associate Professor Ming Ye was selected as a 2012 recipient of the Department of Energy Early Career Award. The Early Career Research Program supports the development of individual research programs of outstanding scientists early in their careers and stimulates research careers in the disciplines supported by the DOE Office of Science. Ye was one of only 68 selectees chosen based on peer review of over 850 proposals and the only person chosen for the award from FSU. The award was made through DOE's Biological and Environmental Research program, whose mission is to understand complex biological, climatic, and environmental systems across spatial and temporal scales. The office encourages exploration of the physical, chemical and biological drivers of climate change, and seeks the geochemical, hydrological, and biological determinants of environmental sustainability.

The goal of Ye's research proposal, Computational Bayesian Framework for Quantification and Reduction of Predictive Uncertainty in Groundwater Reactive Transport Modeling, is a greater understanding of subsurface environmental systems. These systems are inherently open, complex and dynamic. Understanding and predicting system responses to natural forces and human activities assists scientists, practitioners and policy makers in managing water resources, cleaning subsurface contamination at DOE sites, and providing expert analysis and long term stewardship of nuclear waste disposal and CO2 storage facilities.

"When contamination occurs, it's difficult to pinpoint the time when the contamination occurred, and going back and calculating the time that the contamination will last is difficult. The calculation, however, is important to do because you need to know how large the contamination site is, the source of the contamination, the substance(s) involved in the contamination, what kinds of other substances have interacted with the site since the contamination – those kinds of things. Sampling is limited because it's costly. Some testing is done, but again, it's limited, so it's not enough to obtain all the information you wish you had. In order to do this properly, you have to know how, when and where to test. To reduce the risks of failure and use the proper test and testing methods, you have to know or have a good idea of what the test is likely to produce."

Ye plans to combine methods to mitigate uncertainty and create a cohesive and inclusive model. "I plan to use a comprehensive, systems-based Bayesian framework and the sparse grid methods that were developed here at the department by Max Gunzberger and his group. This approach will address model fragmentation currently found in uncertainty quantification, and diminish the current error propagation rate that inevitably occurs when measurement processes or model scales are combined."

"Sometimes we make an educated guess about what will happen at a contaminated site, but we don't always know. For example, at the DOE Hanford site in Washington state, we thought the contaminants

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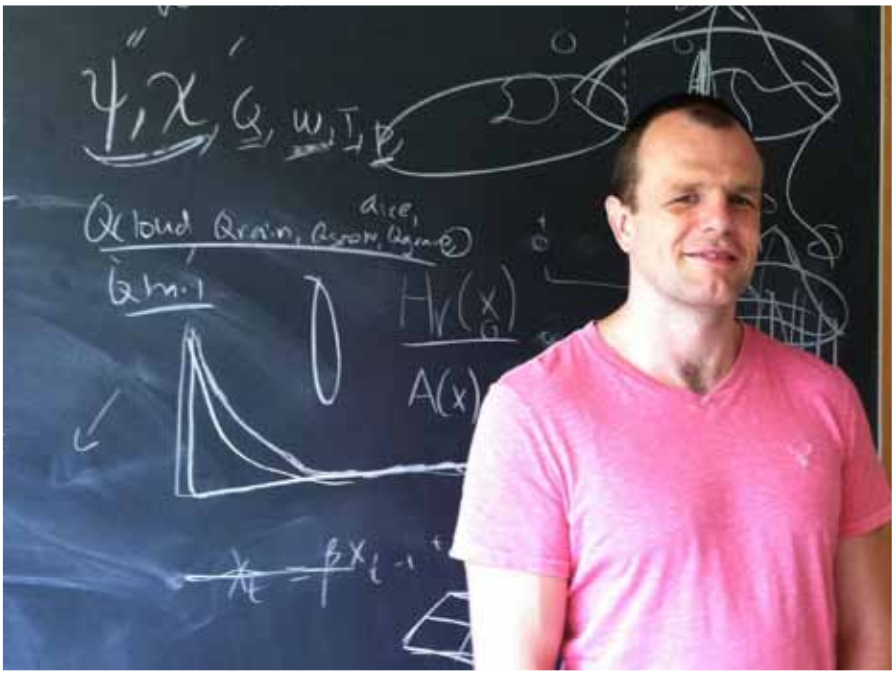
Palczewski creates encryption software



Ph.D. student Michal Palczewski

An unexpected email led one Scientific Computing student to an internship opportunity and the creation of a software that will assist the Federal Bureau of Investigation, police and other law enforcement agencies in maintaining secure data transmissions. SC doctoral student Michal Palczewski attended a Datamaxx mixer and recruiting event after receiving an email from Assistant Professor Sachin Shanbhag.

"I got an email from the department about this recruiting event at this company called Datamaxx – they called it a lunch and learn. So I thought, 'Let's see what's out there.' So I went there, even though I didn't really know what to expect. I just thought it would be interesting."

When he attended the recruiting event, Palczewski had already written two apps for the Android. The first one was an app that provided additional features to mobile devices that were connected to the FSU wireless network. The second app was a task manager, and both were available for download.

"So I go there and I start talking to people and they ask me about what I do. I told them I've been programming for Android devices. I had an Android phone, and just as a hobby on the weekends I would write apps. I'd written two apps that were available for download, and I'd just pull out my phone to show them while I was talking to people."

While at the mixer, Palczewski was introduced to Bill Lake, Vice President of Software Development. Afterward, Datamaxx hired him and let him choose whether to write software for the iPhone or the Android.

"When they asked me whether I wanted to develop for the Android or for the iPhone, I decided to try something new so I picked iPhone development and have been doing that kind of work ever since. I've been working with Matt Burke, a Datamaxx employee, and April Byrne, another intern who is an undergrad student in Computer Science."

For this project, the company wanted to create an instant messaging program that could be used by law enforcement agencies. Because of confidentiality and security, there are specific, strict encryption requirements, and it was imperative the program have FIPS140-2 compliant encryption. FIPS140-2 is the current U.S. government cryptography standard for IT products issued by the National Institute of Standards and Technology (NIST).

"Police and military organizations require a certain level of encryption for their communications, otherwise they're not supposed to use it. Before we created this software, there was no way to do this type of encryption on the iPhone."

Along with Burke and Byrne, Palczewski created an iPhone app that adheres to a U.S. government computer security standard used to accredit cryptographic modules. Palczewski had never heard of this encryption before beginning this project.

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would attenuate over time, but it turns out that they didn't. They simply dispersed horizontally."

"It really comes down to the questions, 'How much confidence do you have that the model is correctly predicting the true error rate?' 'How sure are you that the confidence intervals are correct?'"

The project will use both computational and real-world models based on Ye's previous research. The physical location is the Naturita Mill and Disposal Site in western Colorado, an old uranium mill that began operating in 1939. The mill was used to store waste from the Manhattan project until 1958, and 138 acres of land and groundwater were contaminated in and around the site. The location has complicated hydrogeochemical conditions which have led to significant predictive uncertainty and the risk of failure in site remediation and monitoring.

"The key component of this research is that it's theoretically general, and computationally adaptive. These characteristics make it versatile enough that it can work with any code that is developed."

Ye will receive $760,000 over five years and was nominated by DOE for the 2012 Presidential Early Career Award for Scientists and Engineers (PECASE).

For more information, visit:
www.sc.fsu.edu
http://people.sc.fsu.edu/~mye/
http://science.energy.gov/early-career/
http://science.energy.gov/about/honors-and-awards/pecase/
www.geosociety.org

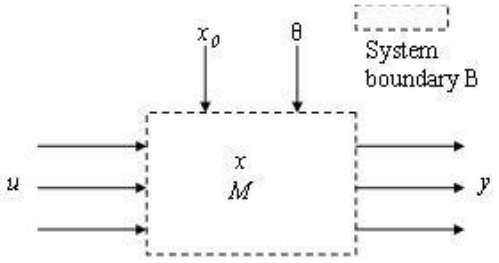

Figure at left: Diagram of model components from a system perspective.

In addition to receiving the DOE Early Career Research Program award, recently Ye was nominated for and selected as a Fellow of the Geological Society of America. The Geological Society Fellowship is bestowed by election only, and is reserved for those most outstanding in the profession. Ye was nominated by Mary C. Hill at the U.S. Geological Survey for contributions "to the numerical simulation of groundwater flow and solute transport in saturated and unsaturated porous and fractured media and to uncertainty analysis and risk assessment using stochastic methods, GIS, and high performance computing."

GSA's newly elected Fellows will be recognized at the 2012 GSA Annual Meeting Awards Ceremony on Monday, November 5, 2012, at the Charlotte Convention Center.

Palczewski, continued from page 2

"It took me about a month or two to figure out how to approach the problem and write the code. First, I did a lot of research into what was required. And we built on a pc-based building block that we found, and adapted it to our needs."

"I was frustrated because I didn't think I could get it work in a way that it would be approved. I wasn't sure it could be done according to the guidelines we had. None of us were. There were moments when I thought it couldn't be done. I just decided I was going to pursue each idea, every possible avenue all the way through to its conclusion before giving up"

The project is near completion, beta-testing is in progress, and they have a time table for distributing it to government agencies for use. Palczewski is looking forward to continuing his work at Datamaxx, as the company has extended his internship, and he is working on new projects.

"I like working in environments with uncertainty and learning new things. I think at one time I would have been less comfortable with it, but this project has been fun, and I'm looking forward to other challenges."

Palczewski's doctoral work is under the direction of Peter Beerli, whose lab seminars focus on understanding mathematical methods and computer implementations in population genetic inferences and phylogenetic inference studies.

For more information about the Department of Scientific Computing, go to www.sc.fsu.edu. For more information about Palczewski and Peter Beerli's research group, go to http://people.sc.fsu.edu/~pbeerli/Beerli_Lab/Group.html.
For more information about Datamaxx, go to www.Datamaxx.com.

Yonsei University students visit for educational exchange

Left to Right: Visitors from Yonsei University - Yoonseop Lee, Jongsoo Kim, Jaemin Shin, Weiwei Fang, and Kyounghun Lee .

GRADUATE STUDENTS FROM SCIENTIFIC COMPUTING'S SISTER department, the Department of Computational Science and Engineering at Yonsei University, visited for four weeks this Summer in July and August. This Summer's visit marks the second time Yonsei students have spent extensive time in Tallahassee at DSC. The relationship between the schools was formally established in early 2011 to promote international cooperation, and facilitate inter-university collaborative exchange. As one of the oldest and most prestigious universities in Korea, Yonsei University is considered one of the two best institutions of higher learning in the nation.

The students' July 7th arrival was strategically designed to coincide with the department's Summer Seminar Series, a month-long succession of introductory information sessions, each one created to present a set of practical skills. Topics presented by SC professors were broad and diverse, and included subjects such as How to make a Mesh, Computational Phylogeny and Evolutionary Biology, and An Inverse Problem in Polymer Rheology.

Opposite page, bottom: Tomek Plewa readies his Summer Series presentation on Reliable Scientific Computing. Plewa's talk took place on July 11th.

In addition to the students' academic pursuits, they spent time enjoying local beaches, visiting the area and to traveling to other U.S. cities. "Our trip to Wakulla Springs and St. George Island was a lot of fun. We saw an alligator. In Chinese, it's a kind of fish that we call 'Èyú'," said Weiwei Fang. While visiting DSC, Weiwei

made the most of her time in the U.S. and traveled north to Atlanta for a weekend with friends. "This is my first visit to the United States. We saw much beauty and many interesting things – trees and many animals, including squirrels and deer."

Jongsoo Kim was intrigued with the methods course offerings available to DSC students. "The first thing I learned was basic random numbers and real random numbers. This was the first opportunity I had to take a class about Monte Carlo methods – I never used them before, I just knew they were used to simulate. I never learned it deeply. We started parallelizing some methods, such as Open MP, Open MPI, CUDA, and Condor and submitting jobs scheduled on the cluster."

"Professor Mascagni taught from several problems that use Monte Carlo methods such as fluid mechanics. Fluid mechanics is my major so I was very interested in that. I never heard of Monte Carlo methods being used for fluid mechanics. Mascagni was studying x-rays. I didn't know there were so many areas using Monte Carlo methods. I am very interested in the material I learned in that class."

"We are not directly using these methods in what I am studying right now. I am studying two-phase theoretical collisions so there is no opportunity to use Monte Carlo techniques, but this is a new area for me, and it's very exciting."

"I was able to learn of lot of what he was presenting in the class. I also attended and enjoyed the many presenters in the summer series. John's [Burkardt]class was every Tuesday and Thursday. They were very interesting and easy to listen to and learn from. I was most impressed with the talk on verification of scientific research given by Tomasz Plewa. I was most curious about the verification process in scientific computing and this is something they were not teaching in Korea. I was happy that I could find classes here that I could not find in Korea. Now I want to come again and take classes here for a full year – classes that I can't get in Korea."

During the final week of the visit, Burkardt and DSC graduate student Detelina Stoyanova enjoyed a farewell lunch with the students, where they talked about their time in Tallahassee, but also their trips to other places. Jaemin Shin went to Chicago, and Kyounghun Lee talked about his visit to New York City where he visited Times Square, the Statue of Liberty, the Brooklyn Bridge, NYU, and Columbia University. "There were so many lights and the lights were so bright there. It was amazing. I walked all day long. I visited museums like the MoMA. I really felt the American life."

Before they flew back to Seoul, Max Gunzburger and John Burkardt presented each student with a certificate marking their time at DSC.

For more photographs of Yonsei students, DSC students, and DSC staff at the beach, go to www.facebook.com/FSUSciComp. For more information about Yonsei University, go to www.yonsei.ac.kr/eng/.

"I was happy that I could find classes here that I could not find in Korea. Now I want to come again and take classes here for a full year...."
---JONGSOO KIM

Exiting student lands plum position

While many recent grads are looking for work long after graduation, SC doctoral candidate Nathan Lay received and accepted a position at Siemens Corporate Research in Princeton, New Jersey, even before completing the final steps of the degree. The job offer followed a summer internship in New Jersey, where Lay worked with Jingdan Zhang on a successful image segmentation project. Nathan began his full-time permanent position in May.

Both of Lay's professors, Anke Meyer-Baese and Adrian Barbu study medical imaging and image segmentation, and Barbu is a former Siemens employee who told Lay about the internship position and recommended him for it. Barbu was glad to help Lay obtain the postion and believed it to be a good fit with his skills.

"Nathan is passionate about research, hardworking and driven by an unquenched curiosity. He has a very good command of numerical methods and programming, which helped him advance past many obstacles in his research. I am very happy with the work he has done and am sure he will do very well in his career," said Barbu.

After seeing Lay's work during the summer, Siemens extended the offer for permanent employment.

"Adrian told me about Siemens several times while I was doing my graduate coursework. After the summer, Jingdan Zhang, my supervisor at Siemens, said everybody was really impressed with the work I did up there. I did quite a lot of work, and they wanted to hire me because of that."

One of the things Lay did during his summer internship that impressed his new employer is he co-created a new and fast simultaneous multi-organ segmentation system based on regression rather than Marginal Space Learning. This system achieved a 10x speedup with competitive accuracy compared to the current state-of-the-art system. Lay also programmed new features, bug fixes and contributed a new classifier to their current framework.

"They were very happy with the image segmentation acceleration. I think they may want to do segmentation as close to real time as possible. They want responsiveness. They give this application to customers, so this could be important to customers depending on their needs. If you could do segmentation in real time I can imagine there could be a lot of useful applications for that. Also I just think the responsiveness gives the customer a better impression and could possibly help the customer be more productive. I can think of some examples of possible situations. Let's say you're segmenting 10 organs in a volume and it takes you two minutes, as opposed to some longer time frame. Or perhaps they are able to use the segmentation in some automated fashion. Being able to accomplish that faster or as close to real time as possible could be very attractive depending on what the customer is trying to do."

Ph.D. student and Siemens staff Nathan Lay

"Siemens is interested in applications that are applied and immediately useful, and Lay credits many of the things he learned as a DSC student with helping him gain the skills necessary to be successful at Siemens. "Scientific Programming, the Intro to HPC course, the machine learning course, ACS1 and ACS2 were all very relevant to my internship. You need a very strong C/C++ background to work at Siemens Corporate Research as well as exposure to other kinds of development and miscellaneous tools (for example, cmake, matlab). DSC courses generally expose the students to a wide array of development tools. Elec-

tive courses, such as Intro to HPC, also provide a lot of insight of how to speed up applications. Speed is very important for this kind of application."

As for living and working in the northeast, Lay is from Boca Raton, Florida, and liked the Princeton area right away. "When I was in Boca, there were fewer people, and I liked the bucolic feeling of the place. I like smaller cities because they have fewer people, are quieter and less crowded, and the people in small places seem friendlier. Princeton has a lot of parallels to Tallahassee – they're both small, college towns. In fact, there's a farm right across the street from where I'll be working. I bought a bicycle, and can get around easily by bike in Princeton. I'll be able to ride my bike to work, and the grocery store is only a few miles from where I'll live. Roads and drivers are especially safer in Princeton and Plainsboro, NJ."

Lay began as an FSU undergraduate student majoring in Pure Mathematics, and is looking forward to defending his dissertation and having school behind him. "I've been at FSU for nine years. I started with the undergraduate program in Math. I have to finish the dissertation so I'm not finished yet, but I'm very close."

For more information, go to www.sc.fsu.edu or www.usa.siemens.com/en/about_us/research/home.htm.

Front: Detelina Stoyanova, Cameron Berkley, Brian Corner, Kathryn O'Donnell Miyar, and K. James Soda
Rear: Benjamin Pomidor, Jeff Hudson, Greg Zehner, and Dennis Slice.

Slice Group to study head shape with Army

Dennis Slice and his research group will use three-dimensional surface scans of the head and face to increase safety for U.S. combat soldiers, thanks to a 14-month, $271,000 contract from the U.S. Army Natick Soldier Research Development Engineering Center in Natick, MA. Slice is developing new methods to estimate head surface by using face and forehead geometry. These methods will be beneficial for creating helmets that fit better, and provide higher levels of protection for soldiers in the field.

Three-dimensional scans of the body are common, and can produce true body surface images as long as the clothing worn by the subject is spare and form fitting (think spandex bicycle shorts). Accurate scans of the head are more problematic, however, as hair obstructs the scanner in capturing an accurate image and true shape of a head. Wearing a cap can help, but doesn't altogether eliminate the impact of hair in the image, especially for women and people with thick, curly hair.

Slice, in collaboration with the Anthropology Team in Natick and others, will examine the problem using traditional variables such as distance and angles, 3-D US Army inputs, and other anthropometric elements to build a statistical method for estimating full head surface models based on face and forehead anthropometry and geometry.

The research will have a strong impact on all protective headgear including sports helmets (football, hockey, lacrosse), bicycle helmets, motorcycle helmets, to name a few. The medical community will benefit as well. Three-dimensional surface scans are often utilized to guide the creation of protective headgear for patients recovering from head surgery or to protect individuals whose head shape is outside of standard norms.

For more information, go to http://dslice.site.aplus.net/dslice/index.html.

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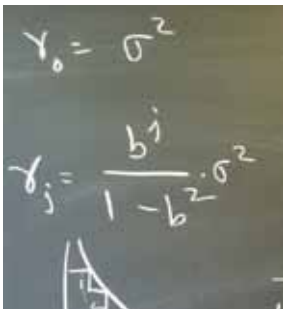

There's so much more to see at our Facebook page! Visit is at www.Facebook.com/FSUSciComp.