Department of Scientific Computing
Fall 2012

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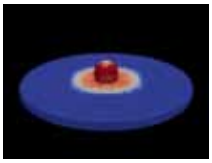

Gunzburger awarded Rothschild Fellowship at Isaac Newton Institute

As part of its commemoration of the Year of Climate Modeling, Frances Eppes Professor and Scientific Computing Chair Max Gunzburger was invited to the Isaac Newton Institute for Mathematical Sciences at the University of Cambridge. Gunzburger was the Rothschild Distinguished Visiting Fellow for the event and the keynote lecturer for the Multiscale Numerics for the Ocean and Atmosphere series. He gave a special lecture entitled, *The Science of Ice Sheets: The Mathematical Modeling and Computational Simulation of Ice Flows.*

"The ice sheets presentation was a special lecture – part of a special program that they had on climate modeling. They had a lot of people there, and everybody talked about their own research," said Gunzburger. "I gave two other talks – those were more focused on ocean and atmosphere. I had to give a special lecture for the Rothschild fellowship – that's what I did on ice sheets. The others were more specialized to people who were in this program, but the Rothschild lecture was more general, and was for anyone who might be interested in that topic."

Gunzburger spent September and October in Cambridge at an extended research forum designed to immerse scholars in an atmosphere conducive to idea generation and collaboration. Climate system models consist of ocean, atmosphere, sea ice, land ice, and land. Each of these components are studied separately by different research groups in different parts of the world. Gunzburger selected the science of ice sheets as a topic, due to its complementary and continuously developing role in climate modeling. The subject is also particularly relevant to the U.S. and to Florida.

"If you want to talk about climate and model ice sheets, you have to look at the amount of fresh water in the world. Seventy percent of the fresh water in the world is Greenland and Antarctica. Most of the rest of the 30 per cent is underground. So what's on the surface – lakes, rivers – is just a very small percentage. So the only thing that really counts when you talk about melting ice sheets is Greenland and Antarctica as far as sea level rise is concerned."

"One of the things scientists talk about when they discuss global warming is a concern about sea level rise. Florida is flat and low lying, and has the lowest highest point in the nation. Its highest point is Britton Hill which is 345 feet, and Sugarloaf Mountain is the highest interior point in Florida at 312 feet. If there were a six meter sea level rise, much of south Florida and all of the coastal regions of the state would be under water. So sea level rise is especially relevant to Florida."

Even though much research exists on climate and climate change, the research is far from concluded. In fact, when it comes to modeling ice sheets much uncertainty

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Message from the Chair

Another year has gone by, and our department has grown its number of students, consolidated its course offerings, expanded its infrastructure, and continued its leading-edge research. To top it off, we just completed our first Quality Enhancement Review.

In 2012 we established a minor in Computational Science, along with a new course offered to the students in the Department of Psychology to help improve their skill sets in a difficult marketplace. Our flagship undergraduate courses, Game Design and Introduction to Scientific Computing, continue to garner interest across a range of departments at FSU.

Without a doubt, the job prospects of our students improves markedly with a course program that emphasizes a mix of computing and practical applications, which defines computational science. Several of our graduate students have graduated this year with Masters and Doctoral degrees, and their education integrating mathematics, computing and applications has helped them land top-notch jobs. Nathan Lay is now at Siemens working on image segmentation for medical imaging. Andrew Young accepted a job at Sony, and is working on software to conduct automatic testing of software packages in development. Doug Jacobsen and Geoff Womeldorff are postdocs at Los Alamos, and Geoffrey Miller is an instructor at FSU. Dan Lu received a postdoc from the US Geological Survey. Other jobs landed by our students include Research Engineer at Outbrain, and research scientist at KAUST (in Saudi Arabia). We are very proud of Ph.D. graduate Guannan Zhang, who received the very prestigious Householder Fellowship at Oak Ridge National Laboratory.

Last summer, SC welcomed five students from Yonsei University in South Korea, from the Department of Computational Science and Engineering. The students took a variety of classes not given in Korea, including monte carlo methods, parallel algorithms, and validation and verification.

One of the more notable achievements includes that of Michal Palczewski, who, during an internship, developed a high level encryption software system for the iPhone, which will be used by the FBI.

Three of our faculty, Ming Ye, Xiaoqiang Wang and Sachin Shanbhag, were awarded tenure and promotion. Ye was awarded a DOE Career award and tenure, while Wang and Shanbhag received tenure and promotion to Associate Professor.

Max Gunzburger, department chair, was awarded the Rothschild Fellowship at the Isaac Newton Institute at the University of Cambridge, where he spent some time working on Climate modeling, specifically issues relating to sea level rise, of particular concern in Florida.

Faculty research continues to be recognized nationally. In total, faculty was awarded more than four million dollars over the past year from the National Science Foundation, the Army, and the Department of Energy, a testimony to the creativity and relevance of their research activities.

We have upgraded our infrastructure in the last year by replacing the main classroom computers with the latest high quality equipment and we acquired a 65" 3D Smart TV screen for interactive presentations with a video-conferencing component. The department contributed funds to the HPC buy-in, supplementing contributions from Peter Beerli.

Finally, our first Quality Enhancement Review gave us the chance to perform a deep introspection at all levels. The Review determined the department is on sound footing with a growing undergrad program, a stable graduate program and a strong curriculum.

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remains, and predictions vary according to what climate model is used.

"An important thing to note is that there's this group that won the Nobel Prize at the same time Al Gore did – it's this international panel, IPCC, the Intergovernmental Panel on Climate Change. They put out a report every seven years about the state of the climate. The last one was in 2007, and of course, one of the things people are interested in is sea level rise. The IPCC refused to make any predictions about sea level rise because they said the science of ice sheets on Greenland and Antarctica wasn't good enough to make a science-based decision. This is after they take all the computer models of climate in the world – there are about 23 of them – and run the same problem with the same conditions and see what the models say. They look at what the differences are in the prediction. What they found last time is the models were all over the place due to the fact that they weren't modeling Greenland and Antarctica well. So there's still work to do."

This trip marks the second consecutive year Gunzburger was invited to participate in this kind of international forum. Last year, he was a visiting fellow at the Oxford Centre for Industrial and Applied Mathematics at the University of Oxford.

Based at the University of Cambridge, the Isaac Newton Institute for Mathematical Sciences is a national and international visitor research institute that organizes and presents research in mathematics and the mathematical sciences with applications over a wide range of science and technology topics. It attracts leading mathematical scientists from the United Kingdom and internationally, to interact and exchange research ideas over an extended period.

Young accepts Position at Sony

SC GRAD ANDREW YOUNG

The day after defending his master's thesis, recent SC grad Andrew Young packed up his things and headed across the country. Young's skills were in high demand during the close of his academic work, and he had a desirable position waiting for him after graduating in August.

Immediately after posting his resume on Dice.com, Young was contacted by recruiters from many interested companies. Dice.com is a career site for technology and engineering professionals that specializes in matching employers with experienced and highly skilled technology and engineering job candidates.

"I received several opportunities in business programming, but the offers that interested me the most were from Dreamworks and Sony," Young said. "Both companies were interested in my ability to work on graphics programming and the computational math I learned at SC."

Young accepted a position as Software Quality Assurance Engineer at Sony Computer Entertainment located in Foster City, CA, a city frequently cited as one of the best places to live in the U.S. Sony is one of the ten largest employers in the area. Young's first project is writing software which attempts to automate testing of other software packages in development.

"The ability to work with graphics programming in a great location was the most appealing factor. I believe the research I did helped me the most, because I was allowed to explore many areas independently. I learned many of the skills necessary for my job including OpenCL, OpenGL, and C++ programming. "

Young committed to a one-year assignment with Sony, and at the conclusion of the year, expects Sony will either offer him a permanent position or an extension of the contract. Regardless of what Sony may offer, Young is already thinking about and planning for the future. "It's hard to know my plans after the contract period. I still have offers come in on occasion. My decision will be based on whether I still enjoy the work after a year."

SC Affiliate publishes in RSS Journal

Long-time SC affiliate Dennis Ridley has a forthcoming article in the Journal of the Royal Statistical Society, one of the world's oldest journals. Ridley's article is slated for Series A of the journal, Statistics in Society, and will appear in the Fall edition of the journal.

Ridley's article proposes antithetic combining as a means of reducing bias in models of serially correlated data. In the model, antithetic time series analysis is used to retrofit a given time series model, with the objective of reversing and eliminating bias in the extrapolated values. By applying antithetic combining to the best single model, values that are perfectly negatively correlated with the original fitted values are produced. The original and antithetic fitted values are then combined, such that their systemic error components dynamically cancel. The method causes forecast error variance to be reduced to a constant, rather than becoming serially and cumulatively larger. Former SC postdoc Pierre Ngnepieba is the article's co-author.

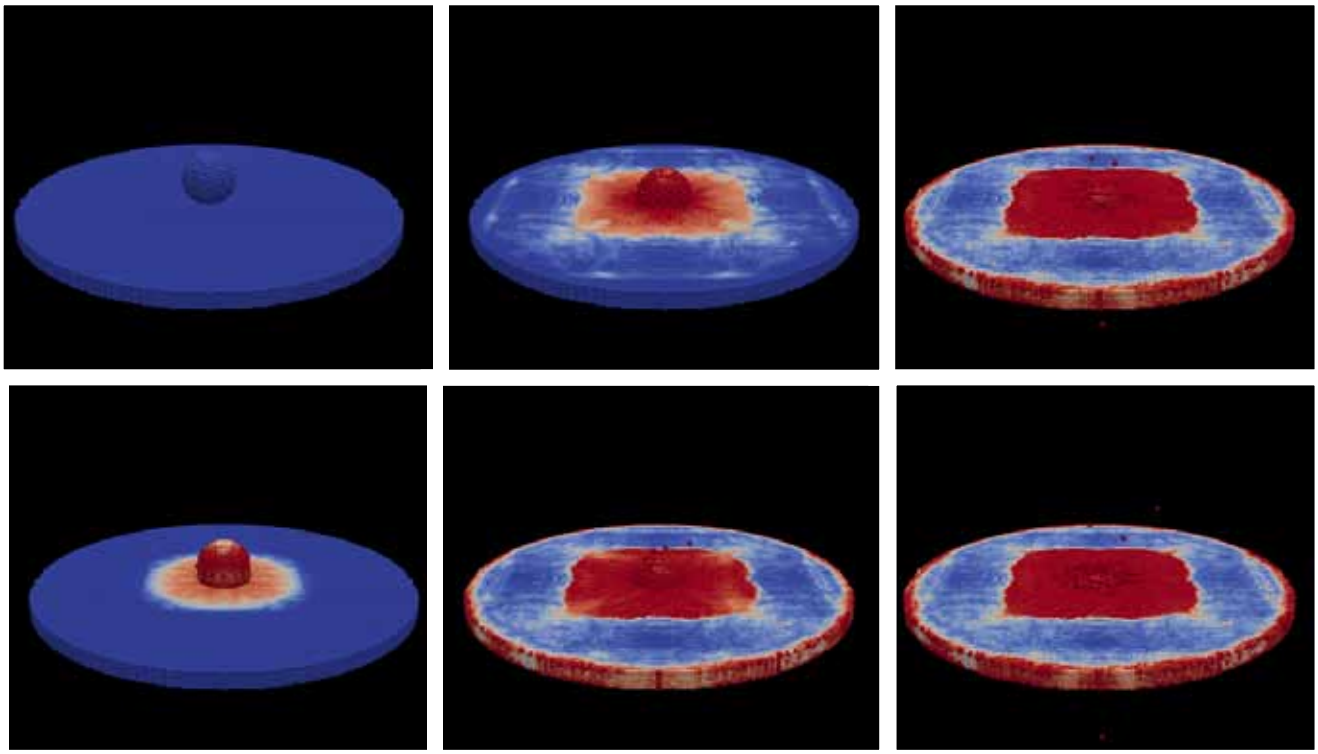
"There are many important applications in all areas of science, not the least of which is climate modeling that investigates what has become known as global warming. The smallest bias will accumulate, so much so that conclusions may be as much an artifact of the mathematical model as they are about climate dynamics," said Ridley.

"This is a commonly known issue with serially correlated data. Not having to correct for the bias in the parameters - only the extrapolation - was, I think, one of the key factors in the research. This research doesn't fix the parameters, though. Now, my next job is to see whether I can correct the parameters. Researchers may use the values of the parameters themselves. The parameters constitute an impulse response function that is used in the study and design of loud speakers, digital filters, electronic processing, control systems, acoustics, and economics."

The Royal Statistical Society was founded in 1834 and is both a learned society for statistics and a professional body for statisticians. The Society has more than 7000 members around the world and is active in a wide range of areas relevant to the study and application of statistical methods.

For more information, go to www.rss.org.uk.

Shanbhag's Rheology Research has many Applications



Images are various views of a brittle disk that is being fractured by a high speed impactor. This time sequence shows the developing fracture as the impact progresses. Each glyph represents a material point, and the color indicates a damage measure (blue particles are intact, red particles completely decoupled). In this sequence, particles are laid out as a simple cubic lattice.

Since getting his Ph.D. in 2004, award-winning scientist and associate professor Sachin Shanbhag has devoted his research to rheology, the study of how matter flows and deforms under applied force. Shanbhag began his work on rheology in graduate school at the University of Michigan, and has continued his scholarship on how polymers behave at the nanoscale, the size at which fluctuations in average properties begin to have a significant effect on behavior. "There is one problem I have been interested in for a while, which is using molecular dynamics to model really small systems, nanoscale systems, atomic systems. If you have a big computer, you may be able to analyze a million atoms, but a million atoms is nothing. For example, two grams of hydrogen contain 10^{23} atoms. That's a huge number – that's like a trillion trillion! That's how many atoms you'd have to use to realistically model two grams of hydrogen."

Molecular dynamics can be broadly applied in research. It is used in creating new drugs, discovering the nature of viruses, and comparing the properties of solvents. As long as materials are relatively homogenous, it can be used to simulate how atoms and molecules interact, approximating their movement. It may seem counterintuitive, but modeling systems at an atomic scale can advance research for critical large scale infrastructure projects such as in Shanbhag's current research. "Ultimately, what we're really interested in is in modeling things like bridges or aircraft, so we're talking about somewhere on the order of meters and kilometers. If we use relatively standard materials like steel to build aircraft and bridges, so long as the material is relatively homogeneous, we have a pretty good handle on how to model them. But increasingly, and this is true of automobiles, and definitely in aircraft and space, a lot of metals are being replaced with polymers or polymer composites."
Introducing polymers and polymer composites in manufacturing provides many advantages. Polymers such as polyethylene excel in contributing characteristics such as stiffness, strength, durability, consistency, malleability and resistance to objects. Even so, there are disadvantages, as plain polymers such as polyethylene and rubber soften or degrade when exposed to heat, light and air. Polymer composites, though, can mitigate some of these issues by incorporating other elements.

"So in automobiles or aircraft, the ability to perform well in high temperature environments is important. And plastics by themselves don't work. You need them to be impervious to the physical elements or they don't meet performance standards or expectations.

Consider carbon fiber, which is pretty ubiquitous these days, it really is a carbon fiber polymer composite. They take these carbon fibers, and they stick them in a polymer. This gives you a lot of the advantages of plastic because it's light, it's easy to process, it's highly malleable and can be made into all sorts of different shapes without any decrease in integrity. In metals especially, shaping is not easy but plastic is easy – you can blow it, you can push it at high speeds – it can do all sorts of things. And then it's much cheaper than metals. The shapes you can create and the energy required to make those shapes is really very small. These composites really marry the best of both worlds. You get strength, durability and an ability to withstand temperature with these inorganic fillers.

"What has happened recently is people have discovered carbon nanotubes and nanoparticles. These nanotubes are like a carbon fiber except they're very, very small and they're super strong. Pound for pound, it's like a wonder material. It's several times stronger than steel. It's very conductive – it's more conductive than copper, for example. It has a lot of very desirable properties. So people have wanted for a long time to mix these types of materials in a polymer matrix instead of carbon fibers. The idea being that carbon fibers by themselves are heavier than polymers so when you make a traditional polymer composite, they still tend to be heavy. They're much lighter than steel, but heavier than you want them to be. The idea is if you can use very little of these carbon nanotubes instead of the carbon fiber, you will get a lot of improvement in the mechanical properties, but you also open up a completely new set of possibilities because of their electrical applications and other conductive properties."

One new possibility being studied by Shanbhag and Steve Henke, his doctoral student, with collaborators in the industrial engineering department, is using carbon nanotubes as sensors. These sensors would serve as an early alert system and could avert large-scale disasters. "For example, one thing people use them for is if you can make sensors. People can place the carbon nanotubes in a thin film of a polymer matrix, and because it's conductive, it conducts just like a wire; its dimensions are about a nanometer in width and about a micron in length. But if you put the tubes adjacent to each other and then pull the matrix, the tubes shift and you can measure the change in conductivity, you can measure the electrical signal that shows how much things have shifted. So let's say you want to make these sensors and place them in highly sensitive places on an airplane or a bridge – maybe in the form a cellophane tape. If any part of the bridge has any structural damage, and something about the bridge shifts, we could measure that something has shifted. Since we know the location, we can find out which part of the bridge or which part of the aircraft may have been compromised without needing any physical or visible change. So maybe before a wing falls off, the sensor could potentially measure and perhaps give us the chance to repair or prevent large problems. If you catch things early while the damage is small, you can potentially prevent catastrophe. This is true with many things – earthquakes, cancer screening, that's true everywhere. If you catch it early, you have a much better chance. That's one application of these materials."

> "Before the big things happen, small things happen."
>
> ---SACHIN SHANBHAG

New Graduate Students & Postdocs at Scientific Computing

Bacim Alali, SC Postdoc

Bacim Alali studied as an undergraduate in Jordan at Yarmouk University, and as a graduate student at Louisiana State University in Baton Rouge. He received the BS in 1998, the MS in 2005, and took the Ph.D. in 2008, all in mathematics. He has taught and published in mathematics, and in addition to positions as a Software Programmer/Developer at Zeine Technological Applications and a Research Mathematician at Estarta Solutions, he held the Ed Lorenz Postdoctoral Fellowship at the University of Utah. His research is in multiscale analysis with multiple applications, including the mechanics of heterogeneous media, optimal design of composites, fracture and fragmentation in materials, mathematics of climate, and image analysis. Currently Bacim works with Max Gunzburger on multiscale nonlocal theories.

Bacim coaches youth soccer, and plays soccer and basketball in his leisure time. He is married and is the proud father of three - Ahmed, Ibrahim, and Hatim.

Kuo Liu, SC Postdoc

Kuo Liu grew up in Chengdu, the capital city of Sichuan Province in southwest China. She received the Bachelor of Science in mathematics from the University of Science and Technology in Hefei in 2007, and expects to receive the Ph.D. from the University of Colorado at Boulder in December 2012. While in Boulder, Kuo worked in the public and private sectors as an intern and research assistant, studying high order finite element methods, developing algorithms, implementing parallel code using the PETSc library, and modeling physics problems. Kuo worked at NCAR, the UC-Boulder Department of Applied Mathematics, and at Tech-X Corporation.

When away from her research, Kuo enjoys running on trails, watching the seasons change, enjoying microbrews, drinking good coffee, and singing. She is enthusiastic about the Tallahassee running opportunities, and is learning the local trails.

Kuo's current research on peridynamics is supervised by Max Gunzburger.

Hans van Wyk, SC Postdoc

Hans-Werner van Wyk is a 2012 Ph.D. graduate of Virginia Polytechnic University in Blacksburg, VA, with undergraduate and masters degrees from the University of Pretoria, South Africa.

Long active in mathematics research and professional organizations, Hans is a member of the American Mathematical Society, and past president of the VT chapter of SIAM. His research interests lie in the use of variational methods in control and parameter identification problems when the parameter to be identified or controlled is uncertain. Other interests include numerical and functional analysis, statistics and probability, reduced order modeling, robust control, optimization, and mathematics of finance.

In addition to his research, Hans has taught undergraduate courses in mathematics, and advanced calculus courses to high school teachers and teachers in training.

Hans is working with Max Gunzburger.

Huaiwei Sun, SC Postdoc

Huaiwei Sun studied as both an undergrad and graduate student at Wuhan University in China, receiving his Bachelor of Science and Ph.D. in Water Resources and Hydrology in 2006 and 2011, respectively. Before coming to Scientific Computing, he was an Assistant Professor at the School of Hydropower and Information Engineering at Huazhong University of Science and Technology.

Huaiwei's research interests are in water resources and hydrology as they relate to soil water, groundwater and water environment occurring from agriculture. His expertise is in modeling hydrologic events, their effect on soil saturation, solute transport, water flow, salinity, and irrigation. He has published his research in journals such as Transactions of the CSAT, the Journal of Irrigation and Drainage, and the Journal of China University of Geosciences.

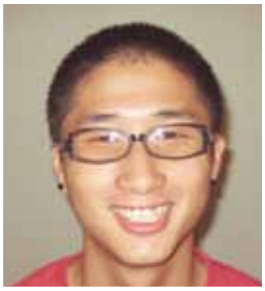
Hauiwei is working under the direction of Ming Ye.

Philip Boehner, Ph.D. Student

Philip Boehner hails from Aiken, SC and received his undergrad degree in physics and pure mathematics in May 2012 from the College of Charleston in South Carolina. In a previous research project, he worked on building a relatively simple simulation that had the end goal of finding the contribution cloud cover has to the overall amount of light that enters the atmosphere from a microphysics point of view. Philip used a combination of monte carlo and ray tracing techniques to find how entering photons interact with individually placed particles in a cloud volume.

Although much of his time is consumed with school, Philip likes to browse the internet and watch sci-fi shows on Netflix.

Philip is a member of Sigma Pi Sigma, the National Physics Honor Society.



Buyun Yang, Ph.D. Student

Originally from China, Ph.D. student Buyun Yang received his undergraduate (May 2011) and Master of Science (May 2012) degrees from Tulane University in New Orleans, where he studied Mathematics, Physics, and Computational Science. Buyun's research includes numerical fluid dynamics, movement of Choanoflagellate in 2D, numerical methods for linear hyperbolic conservation laws, diffusion approximating by random walks, and numerical convergence problems.

Before coming to SC, Buyun was a Research Assistant and Time & Motion Study Analyst at Tulane, a Marketing Research Assistant for Shaoxing WideTex Import & Export, and Associate Director of Operations at Shaoxing Surmount Education Center.

Buyun enjoys programming and tinkering with machines and electronic devices. His hobbies are working out, basketball, cooking, sleeping, and listening to R&B, rap, jazz and rock music.

Kushal Venkatesh, MS Student

Kushal Venkatesh arrived in Tallahassee from India in August to pursue a MS in Computational Science. Kushal received his undergraduate degree from Visvesvaraya Technological University in Mechanical Engineering and a post graduate diploma in Aviation Law and Air Transport Management from Nalsar University of Law. He holds certifications from the Indian Institute of Science in Introduction to Numerical Grid Generation and Fluid Flow Computations involving Computational Fluid Dynamics and Design Optimization and Structural Analysis of Mechanical Systems involving Mechanics and Strength of Materials.

As an undergrad, Kushal won first prize for designing and modeling an international airport in a competition held in Bangalore. He worked for two years as a mechanical engineer for Firepro Systems and as a Design Engineer at Aero Accessories after completing the undergrad degree.

Kushal likes to play the Tabala, a Hindustani musical instrument, swim and jog.

Daniel Fenn, Ph.D. Student

Daniel Fenn transferred to Scientific Computing as a doctoral student after receiving a BS in physics from Utah State University and spending a year as a grad student at FSU's physics department. Daniel transferred because he found SC's interdisciplinary nature very appealing. Presently he is enjoying SC and would like to continue studying physics and doing research that allows him to continue in that direction.

As an undergrad, Daniel spent several years it the Space Dynamics Laboratory at USU. His research centered on the development of upper atmospheric sensors, where Daniel's primary involvement was in the creation and implementation of computer simulations that allowed extensive theoretical testing and pre-fabrication design modification. Daniel also spent a summer in Greenbelt, MD at NASA's Goddard Space Flight Center.

When he gets a spare moment, Daniel likes to run, hike, play the piano, or ride his motorcycle. He is also learning to play the guitar.

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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 the Interim Chair of the Department of Scientific Computing. He can be reached at 850.644.0143. 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.

C. Pennington, MS Student

Charles Pennington came east to Florida to pursue his masters degree from Colorado, where he studied chemical physics at Adams State College and applied mathematics at Metropolitan State College of Denver. Charles has studied a wide variety of topics, including the birth of the universe, wind and weather prediction, and vehicle aerodynamics.

Charles is imaginative, and likes to consider how making small changes in the past would affect the present and future. His other pastimes include writing, concerts, operas, reading, and television.

Markus Flaig, SC Postdoc

Markus Flaig received his Ph.D. in astronomy and astrophysics in 2011 from the University of Tubingen in Germany. He has taught undergraduate courses in mathematics, physics, theoretical electrodynamics, and quantum mechanics, and his articles on protoplanetary discs and other research are published in many journals, including the EAS Publications Series, HP Computing in Science and Engineering, and Physics Review.

Markus works with Tomek Plewa. He and his wife Yi-fen have a son, Joel.

C. Cruikshank, Ph.D. Student

Christopher Cruikshank is from Pensacola, and received his undergraduate degree in Computer Information Systems from Florida A&M University. His research has included autonomous mobile robotics and computer vision, the application of computational methods to astrophysical particle detector simulations, and control systems automation and design for spheromak based physics experiments.

Christopher has a 9-year-old son, Alex, and enjoys yoga, meditation, gaming, and exercising.

Message, Continued from Page 2

In the coming year, our department will continue to grow, with emphasis on our undergraduate program. We are working on new courses to help a wider number of students throughout the University Colleges to gain an appreciation for how computers affect our everyday lives, and how they are used in practice. We will continue to forge collaborations with departments throughout campus, and will seek to promote the ideas of Computational Science as a discipline in its own right, of increasing relevance in a world dominated by fast-paced changing technology.

Gordon Erlebacher
Interim Chair

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