Department of Scientific Computing

Fall 2009

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Message from the Chair

I've moved my usual missive to the front page because of a very big and exciting development: at its November meeting, the Florida State University Board of Trustees approved the implementation of the B.S. degree program in Computational Science!

Although similar undergraduate degree programs are offered in other countries, including Canada and in Europe and East Asia, this is the first such program at a research university in the United States. Together with the successful Master's and Ph.D. programs in Computational Science that we have been offering for several years, we will now be able to offer training in computational science at all levels.

We in the Department of Scientific Computing are now busy doing what is needed to begin offering the program starting in the Fall 2010 semester. The main tasks we need to complete are the design of the new courses that are part of the program and recruiting students.

Although not yet finalized, an idea of what our program looks like can be found at http://www.academic-guide.fsu.edu under "Computational Science." There, a sample academic map is given as well as information about the new degree program. In addition to core courses, the program offers students substantial flexibility for taking additional courses offered

by the Department as well as courses offered by other departments. Students will not only obtain theoretical knowledge about algorithms for scientific computing, but will also gain extensive hands-on experience in the implementation and application of such algorithms. In addition, all students will participate in seminar and practicum courses that will involve them research experiences.

Recruiting students into the new degree program requires that we inform a variety of people about what the program is about. We will be letting high school, community college, and FSU students and their advisors and counselors know why the new degree program is well suited for students interested in computers and in one or more of the sciences.

Subsequent newsletters will provide additional details about the new B.S. program and updates of our progress towards its implementation. I close by stating that maneuvering the new degree program

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Plewa Studies the Stars

In a very literal sense, Tomek Plewa's research is out of this world. Plewa's main research interests are problems of theoretical and computational astrophysical fluid dynamics. Composed of two separate, but overlapping applications of hydrodynamics, Plewa's research focuses on the way fluids, plasma and gases behave, and how those fluids interact with the environment. Hydrodynamics is the branch of science that deals with the dynamics of fluids in motion. Studying the way fluids respond to a certain set of conditions is useful in understanding nebulae in interstellar space and in modeling thermonuclear reactors. "Any complex system is of interest to computational scientists," says Plewa, "but having the potential to harness the power of the sun or a star – I find that very exciting."

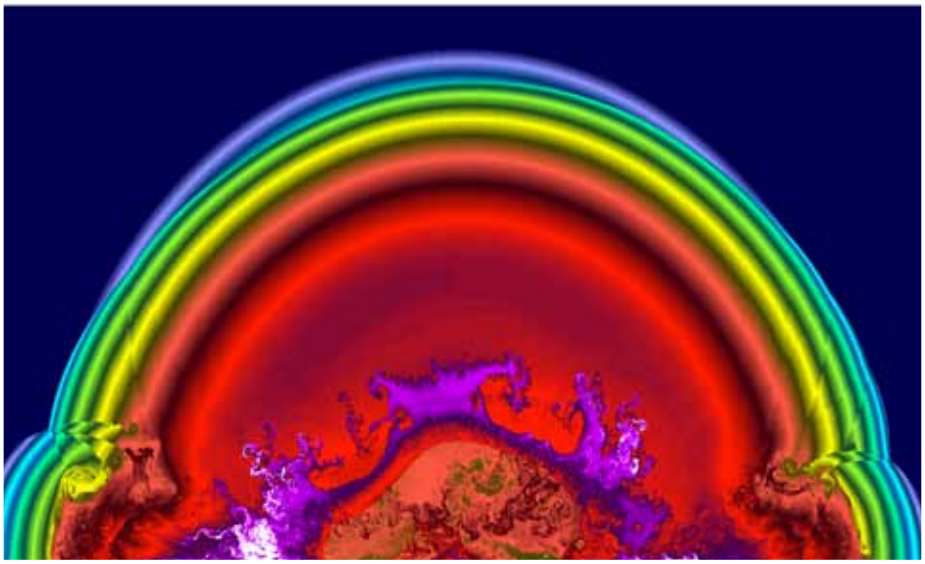

Fig. 1: The supernova structure 6 days after the explosion. The supernova shock is visible as a sharp smooth boundary separating stellar wind (dark blue) from shocked stellar wind (light blue). A complex set of decorations (green) protruding into the shocked wind are Rayleigh-Taylor (RT) "fingers" developing at the material boundary separating stellar wind from the stellar envelope.

How fluids inside a star behave is an important consideration for scientists such as Plewa who do energy research. Stars, including the sun, regulate themselves, and density, temperature and pressure of hydrogen, helium and other gases inside a star increase from the outside towards the star's center. "A star's lighter nuclei can be combined into heavier nuclei in the process of thermonuclear fusion that releases energy. Any process that creates a surplus in energy – energy in excess of inputs – has the potential of addressing global energy needs."

Plewa uses computations to model how external, symmetrical compression helps nuclei to fuse, thereby generating energy. Two processes studied in laboratories, Inertial Confinement Fusion and Magnetically Confined Fusion, use lasers and magnetic field, respectively, to compress and heat light isotopes in a fuel target to generate energy. Many of Plewa's studies are done in conjunction with large research facilities such as NIF (National Ignition Facility) or ITER (International Thermonuclear Experimental Reactor). The equipment needed to conduct these studies is extremely

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through the approval process required the contributions of many in the Department of Scientific Computing, including faculty and staff, as well as the support of the University administration, including Dean Joseph Travis of the College of Arts & Sciences and Provost Larry Abele. I sincerely thank all who helped and supported our efforts in getting the degree program approved.

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complex, built to custom specifications, and used by scientists from all over the world. The models and simulations these machines perform are special, too. "The physics of these models and simulations are similar to recreating the sun in experiments here on earth. Inside a star you find extreme conditions, and the hottest star can be hundreds of times hotter than our sun."

Modeling thermonuclear and core-collapse supernovae present opportunities for possible solutions to intractable global problems such as increasingly fierce competition for energy resources. The simple fact that we use finite resources such as natural gas, coal, and oil so frequently in many of our daily tasks means that over time, their supply will cease. With the growth of large new economies such as India and China, the issue of renewable energy becomes increasingly critical. That makes Plewa's research significant on a global scale, "Access to energy sources is the key to sustaining development and providing global security."

International energy provision isn't the only issue that arises when Plewa talks about his research, as nuclear studies have been the subject of much concern and resistance. "When one says the word 'thermonuclear,' there is a reaction by the public," Plewa says. "People immediately begin to think of Three Mile Island or Chernobyl. The vocal opposition that exists today simply wasn't there thirty years ago."

For now, Plewa and his collaborators continue to work to improve the research that can lead to greater, more diverse energy resources for the planet. For more information, go to http://people.sc.fsu.edu/~tomek/.

New Grad Students and Post-docs at DSC

Although she was born in Louisville, KY, HALEH ASHKI grew up in Iran, where her family moved when she was a child. After completing her Bachelor of Science in Software Engineering at Azad University, Haleh came to the United States to pursue the Master of Bioinformatics at Indiana University. She worked as a software developer, programmer and database administrator in Iran and Indiana, before moving to Tallahassee so she could pursue the Ph.D.

Haleh met her husband Mehdi, a Florida State interior design student, while the two were doing volunteer work for a local charity. Haleh has a number of diverse interests, including cooking and flying, watching the ocean waves, mountain climbing, playing tennis, and hanging out with friends.

HENG DAI returned to his home city of Jinhzhou, China, after completing his undergraduate degree at the University of Science and Technology in Biology in 2006. After working at Yangtze University for a few years, Heng came to the U.S. to pursue his graduate work under the mentorship of Ming Ye. In his spare time, Heng is an eastern Asia history amateur and he likes to watch American movies.

TIM HANDY recently graduated from the University of Central Oklahoma with a Bachelor's in Engineering Physics - Mechanical Systems. Currently, he works for and assists in administering the Condor system. His previous research has been primarily

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Internship Experiences NCAR Research ABERDEEN PROVING GROUND PROGRAMMING Los Alamos National Laboratory C++ PARTIAL DIFFERENTIAL EQUATIONS

Graduate Students Intern Across the Country

Graduate students Jennifer Murray, Geoff Womeldorff, Doug Jacobsen, Steve Henke and Evan Bollig studied in national laboratories during the summer, and experienced research in collaborative and diverse environs.

Jennifer Murray

Jennifer Murray spent the summer developing an algorithm for finding the electronic structure of nanoparticles at the Pacific Northwest National Laboratory (PNNL) in Richland, WA. Nanoparticles are difficult to model because the arrangement of the atoms towards the surface of the nanoparticle becomes disorderly, and the nanocrystal relaxes at the outer edges. In addition, if there are any defects in the nanoparticle, these also become troublesome. "Our solution is to choose representative regions of the nanocrystal and to represent the electron density in Lareas in between in terms of the representative region density. We can do this because we know that the nanocrystal is nearly periodic, and so the electron density is predictable in the areas between representative regions."

Los Alamos morning sky. Photo by Doug Jacobsen.

Jennifer learned methods to solve for the electron density in Density Functional Theory and finite element methods used by computational chemists under the supervision of Dr. Eric Bylaska, Senior Research Scientist in the Environmental Molecular Sciences Laboratory of PNNL.

She also hit the jackpot in terms of living arrangements for the three months she spent in Washington. "Richland is part of a surprisingly small tri-city area. Each city - Pasco, Kennewick and Richland - has its own regional niche that contributes to the area economic and social landscape. You fly into Pasco, shop in Kennewick and the lab is in Richland." Rather than leasing an apartment, Jennifer rented a room from one of the local residents. This alternative proved to be both economical and convenient. "I rented a room for the summer in the basement of one of the local residents. It was really great, because she knew everything I needed to know to be able to find the local attractions and experience the area. I never had that feeling of being a tourist because of her, and I learned a lot about the area. She even took me around on mini-tours of the area to show me the sights."

Geoff Womeldorff

As soon as Geoff Womeldorff arrived in Los Alamos, New Mexico for his internship at Los Alamos National Laboratory, he established a routine around work and leisure. "I would go in to the office at around 9 in the morning. Then I would take a short lunch – maybe five or ten minutes to have a couple of energy bars – then I would get back to my computer and work until 5 o'clock. After work, I would spend time hiking or visiting historic national landmarks – Carlsbad Caverns, Lincoln National Forest, and Jemez/

Santa Fe National Forest."

Geoff spent the first two-thirds of the summer porting a shallow curtain model to CERROS, an accelerator driven concept to produce tritium. In August, he switched gears and began work on a project that may prove to be long-term. "In the third part of the internship, I worked with staff at the National Center for Atmospheric Research doing coding that involved a grid I've been working on that uses their model. I'm hoping we can extend that research into a future collaboration since it's such a good fit."

In addition to the programming and collaboration, Geoff's internship involved regular weekly meetings with his advisors, and access to a student lecture series.

Doug Jacobsen

Doug Jacobsen interned at Los Alamos National Lab in Los Alamos; as it turns out, he bunked with Geoff Womeldorff in student housing at the University of New Mexico, but Doug kept a different, more structured work routine. "I would go in around 7:30 or 8am, then leave at 5pm. I met informally with my mentors (Todd Ringler and Mark Petersen) on a daily basis, once or twice a day – but we had a scheduled weekly meeting, too. Then we had two group meetings every week."

Doug's research for the summer was to explore three separate vertical ocean model grids - two of which are still developmental – to see which one gives the best results for overflow. Doug worked with HyPOP, a new ocean model that has improved methods and parameters for analyzing vertical and depth coordinates of ocean models. In addition to his own research, Doug's fellow group members attended several conference workgroups, then came back and shared their knowledge and experiences. "I can see why people do this kind of research. More parameters create a better model, and I learned a lot about the different parameters and what they mean."

Steve Henke

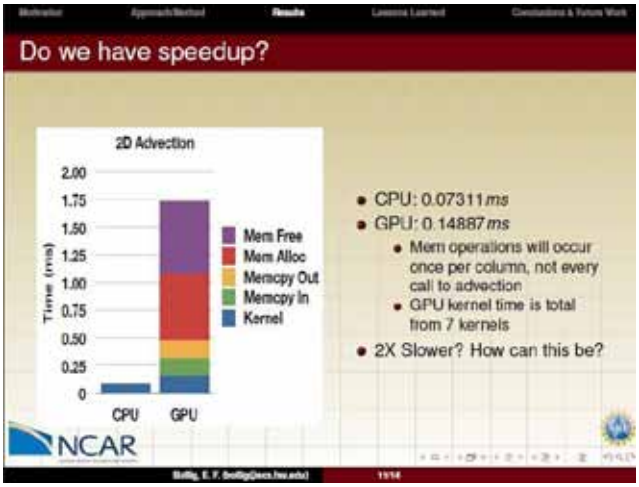
On the other side of the country, Steve Henke interned for a second time at Aberdeen Proving Ground, Maryland where being an intern requires extensive processing, online training, facility tours and demonstrations. Following orientation, Steve concentrated on his research, which involved studying oxide thin film, diffusion, electrostatics, and elasticity. The ultimate goal of the research was to control stability in the morphology of a specific type of film under certain conditions; research like this could have a number of uses in long range communications. Steve worked with DOE code libraries to write finite element method computer code using C++. "The research was an enjoyable aspect of the internship, and living and working in the DC area is very different from Tallahassee. The area has grown so much since I was there last year. It's probably doubled in size, since 2008, so there's a long commute. But there are so many things to do - so many national landmarks and historical venues to see and enjoy."

Evan Bollig

Within two hours of arriving in Boulder, CO to do his internship at the National Center for Atmospheric Research (NCAR), Evan Bollig was hiking the Flatirons on Green Mountain. "I really like Boulder, and the Flatirons were so close! I couldn't wait to get out there." Evan made regular hiking, exploring the city and his research the cornerstones of his summer internship experience. Like many research experiments, Evan began the project expecting one outcome, but actually obtained very different results. "We expected that certain programs and experiements would execute faster on the GPU than on the CPU." GPUs have highly parallel structures that make them especially efficient at running certain complex algorithms.

You can see more photos Geoff and Doug took in Los Alamos, and a presentation of Evan's unexpected results at:
www.flicker.com/photos/peloazul
picasaweb.google.com/Jacobsen.Douglas/LosAlamosSunRise?authkey=Gv1sRgCMrLhbOb1LniOw#/
www.cisl.ucar.edu/dir/09Seminars/Bollig.pdf


Entrance to Carlsbad Caverns. Photo by Geoff Womeldorff



Grad Students and Post docs, continued from page 3

in the area of simulating laminar flow in 3-D micro-bifurcations and other micro-structures in order to determine energy loss characteristics in conjunction with an experimental team.
In his limited spare time, Tim enjoys working on percussion rhythms, engaging in small amounts of engineering and embedded systems programming, playing music games, and sampling fine beers.

Growing up bilingual gave IAN JOHNSON an appreciation for languages, and he has always loved programming and mathematics. Given these interests, it may come as no surprise that Ian obtained a dual undergraduate degree

in Applied Mathematics and Chinese from FSU. Before pursuing his graduate studies Ian worked as a web application developer and he hopes in the future to work on computer vision, visualization and large data sets.
Ian loves the Chinese language, and finds learning and speaking Chinese very relaxing. Currently, he is particularly interested in Chinese character recognition, which helps him continue to increase his language proficiency. Ian also enjoys adventure, travel, open source software, and aquaponic gardening.

Originally from Quito, Ecuador, VERONICA VERGARA LARREA came to Reed College as an exchange student in 2005 from Universidad San Francisco de Quito. A year later, she transferred to Reed and later received her undergraduate degree in Mathematics and Physics. While working towards her bachelor's degree, Veronica studied snow formation and implemented and compared two different algorithms that have been used to model this phenomenon: DLA and Laplacian growth.
Before moving to Tallahassee, Veronica lived in Portland, OR and worked for WebMD Inc. as a software analyst. This experience introduced her to the world of web application development and increased her interest in pursuing a graduate degree. Veronica's re-

search interests include bioinformatics, biophysics, genomics, software and web application development. Some of her favorite things include all kinds of food (especially if it's spicy), dancing, TV, baking, the beach, and movies.

BEN MCLAUGHLIN is originally from Grove City, Pennsylvania, but he is most recently from Lexington, KY. He graduated from Asbury College in 2007, with a degree in Financial Mathematics. Ben's research has been in numerical

solutions of PDE's and numerical interpolation, as well as in macroeconomics. As an SC graduate student, Ben hopes to study additional applications and numerical methods.

When he's away from the department and the university, Ben likes to watch football, play music, dance the Lindy Hop and play frisbee. He's very excited to be part of DSC, and is always up for a second (or third, fourth, etc.) breakfast!

MYRNA MERCED-SERRANO calls the city of Yabucoa, located on the southeastern tip of Puerto Rico, her home. There she attended the University of Puerto

Rico at Humacao and in 2009 was awarded an undergraduate degree in Computational Mathematics. Her degree major was an ideal fit for her research interests, and helped her study biological and material

science applications. Myrna used her background in computation and mathematics to study a hybrid system with ss-DNA and a carbon nanotube. She developed metrics to analyze the trajectories of the simulations and used them to compare the results with metrics available in molecular dynamics packages. In her free time, Myrna likes to watch movies and MTV, her favorite television channel. She also enjoys basketball – in fact, she played four years for her undergraduate alma mater while in Puerto Rico. Myrna's first language is Spanish; stop in and say: "Hola!" any time.

New post-doc JU MING received his Bachelor of Science in Computational Mathematics in 1998 from Wuhan University, one of the oldest universities in China. In 2004, Ju came to the U.S. to study Applied Mathematics at Iowa State University in Ames, Iowa. In June of this year, he completed the requirements for his Ph.D. Ju's primary research interests include optimal control problems, stochastic partial differential equations, and computational fluid dynamics. Currently he is working on Navier-Stokes-Boussinesq systems with stochastic inputs using the sparse grid method, and stochastic partial differential equations driven by colored or white noise. Video games and classical music are two things Ju enjoys as often as possible, given the demands of his research. He's also very happy to be away from Iowa winters and enjoying the warm Florida sunshine. Ju is working with Max Gunzburger.

MICHELLE PERRY grew up in Pittsburgh, PA and received undergraduate (2007) and master's (2009) degrees in physics from FSU. Her research experience is comprehensive, and includes an internship at the Lawrence Berkeley National Lab where she studied neutrinos (2005), a job at Yale at the Wright Nuclear Structure Laboratory studying proton-neutron configuration mixing in nuclei (2006), and work in the FSU John D. Fox Accelerator Laboratory studying neutron-rich nuclei (2004-2009).

Michelle is currently pursuing her Ph.D. and working with Professor Dennis E. Slice. She is working on a project with the goal of developing a 2D digitizer for Morphometrics research, and has been working with the new 3D scanner. For fun, Michelle likes to watch professional football (Go Steelers!!) and national league hockey (Go Penguins!), play soccer, and drink wine and beer. Michelle also loves travel and the arts.

New post doctoral associate MIROSLAV STOYANOV holds dual undergraduate degrees in Computer Science and Mathematics from Concord University in West Virginia, and received masters and doctoral degrees in Mathematics from Virginia Tech in 2006 and 2009. While at Virginia Tech, Miro taught Calculus, and in 2008 he received the Steenek Scholarship for outstanding students in mathematics and statis-

tics. With his previous advisor, Miro developed a number of methods for optimal control of incompressible fluid flow. Currently, he is working with Max Gunzburger on numerical methods for Stochastic Navier-Stokes equations. He is happily married to Zornitsa Georgieva who currently works at Concord University in West Virginia.

ARSIA TAKEH is a native of Tehran, Iran who grew up immersed in science and learning. He received a BS in Chemical Engineering in 2007, and served as president of the Society of Petroleum Engineers while

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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 can be requested from Risette Posey, at 850.644.0196. This publication is available in an alternative format on request.

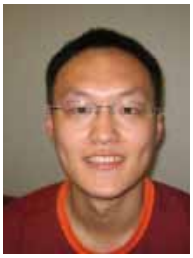
Grad Students and Post-docs continued from page 7

in undergrad. He came to FSU to continue his studies with Sachin Shanbhag. His interests include polymer science, process design, computer-aided programming and mathematics. Besides his academic and scientific activities, Arsia is interested in literature and poetry and has done a great deal of studying in these fields. Mountain climbing, hiking and skiing are his favorite sports.

OLMO SEBASTIAN ZAVALA ROMERO is from Mexico City, Mexico, and got his undergraduate and master's degrees there before coming to Tallahassee to pursue the Ph.D. In 2004, Olmo received his undergraduate degree in Computer Systems Engineering from the Instituto Tecnológico y de Estudios Superiores de Monterrey. After graduating with his bachelor's degree, Olmo enrolled at the National Institute of Astrophysics,

Optics and Electronics in Puebla, Mexico, and completed his masters degree in Computer Science. In previous research, Olmo classified satellite images by using two semi-supervised algorithms based on Expectation-Maximization and Tree Augmented Naïve-Bayes methods. He is considering computer vision, computer graphics and/or machine learning for his doctoral research. Olmo and his wife Yazmin Valdez have been married for three years. Besides spending time together, the couple enjoy different things, including sports (tennis, squash, swimming, volleyball, running, canoeing, and soccer), travel and movies.

GUANNAN ZHANG hails from China, and came to the United States and FSU to do his master's work with Max Gunzburger. Guannan plans to do research on numerical solutions of stochastic differential equations (SDE) and backward SDEs. He received the Bachelor of Science degree from Shandong University in Jinan, where he primarily focused on stochastic computation. Guannan has used his brief time at FSU to organize his home and work lives. He is single,



and in his leisure is an avid swimmer and tennis player. He also enjoys stamp collecting, and hopes to find some excellent additions to his collection.