# Department of Scientific Computing

Spring 2013

CONTENTS



Celebrating Our 5th Year! Department of Scientific Computing 2008 - 2013

## Research group studies methods, games

The development and application of numerical methods and algorithms to investigate, simulate and evaluate fluid flow and heat transfer has always been challenging. The search continues for "the" magical method that requires no or few parameters, is reliable, is accurate and can simulate flows in complex geometries. One such method of interest to SC Professor Gordon Erlebacher is the family of Finite-Difference Radial Basis Function (RBF-FD) algorithms, implemented across multiple CPUs and GPUs. Graphical Processing Units (GPUs) are the video cards found on every computer, which are increasingly leveraged to accelerated computational algorithms running 10 to 30 times faster than on the current generation of CPUs. "The FD-RBF methodology is an algorithm that is, in principle, very simple to implement with data structures that are dimensionality-agnostic. Whether one is solving a problem on a plane or in 3D space, the nuts and bolts implementation details remain essentially the same," said Erlebacher.

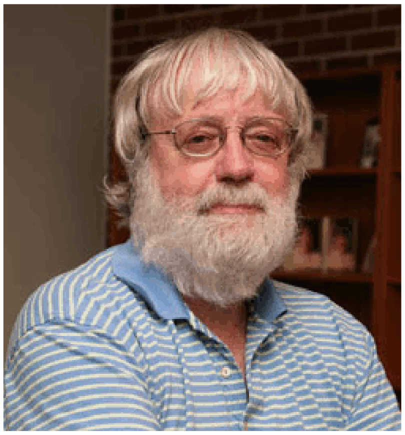
Fluid flow is a form of transport phenomena, that describes the motion of liquid, gas, and other physical processes within a finite physical region, limited by open or closed boundaries. The governing equations for fluid flow are found in many scientific disciplines, including engineering, physics, chemistry, meteorology, and geology.

In the traditional approach, "These radial basis functions extend over the entire physical domain, which guarantees certain desirable properties, such as numerical stability. RBFs introduce a large amount of versatility, because rather than discretize a continuous medium using points that have some structure, radial basis functions allow the points to be placed at arbitrary locations, which is suitable for more complex geometries. For instance, if you're solving for flow in the ocean, the ocean has irregular boundaries and the RBFs can be used to advantage. Of course, it sounds easy, but certain problems that are simple in one context, become more complex in another. Answering a question about the interior of the ocean may become simpler, although handling the boundary may become more complicated." Erlebacher, along with SC doctoral student Evan Bollig and collaborator Natasha Flyer at NCAR, the National Center for Atmospheric Research, hypothesized, then tested and demonstrated a marked increase in utility and speed of RBF-FD on parallel architectures using a combination of CPUs and GPUs.

"Most problems are solved on CPUs these days, but over the last 10 years, GPUs have become increasingly commonplace. GPUs have become cheap commodities, available on almost all personal computers. Of course, GPUs suitable for large-scale computation have more memory, and are more expensive, but orders of magnitude cheaper than conventional processors of equivalent performance. In principle, the GPU can run optimized code 15 to 30 times faster than a single core CPU. Although the original function of the GPU is to run sophisticated games and detailed videos in real time, a wide range of computational algorithms have been developed for the GPU. As a result, every personal computer has become a personal supercomputer running time-consuming applications more than an order of magnitude faster." Using two different architectures, varying stencil sizes and

*See Erlebacher, Page 2*

# Message from the Chair



DSC CHAIR MAX GUNZBURGER

After 18 months on leave and (mostly) away from the job, I am back serving as chair of the Department of Scientific Computing. Over those 18 months, Gordon Erlebacher very ably served as interim chair. I take this opportunity to thank him, on behalf of the Department and from me personally, for the excellent way he handled the rather thankless task of serving as an interim chair. Interim chairs can chose to take one of three paths: they can do nothing and hope the Department does not fall apart, they can do just enough to keep the trains running, or they can make a genuine effort to improve the Department. Gordon not only took the third path, but succeeded in making the Department a better place. It was indeed a great comfort to me, and I am sure to others in the Department and to the University administration, that the Department was in such good hands while I was on leave.

I enjoyed my time on leave very much, which included extended visits to Oxford University, Cambridge University, and the University of Otago in New Zealand, as well as some shorter visits elsewhere. Everywhere I went, I took the opportunity to proselytize the Department so that, hopefully, our fame has become even more widespread than it was already. In fact, I often found that scientists in the far corners of the world had heard of us, but were eagerly curious to know the details of how we operate.

Among the not so pleasant jobs Gordon had to do while I was away was to lead the Department's efforts in connection with the periodic review all departments are subjected to. I am happy to report that, overall, the Department received a very favorable review. For this, I thank the faculty, staff, postdocs, visitors, and most of all, the students of the Department for their effort and dedication to the well being of the Department.

True measures of success of a Department focus on its students, and in this respect, we continue to show very well. Our graduate programs are graduating several Ph.D. and M.S. students, all of whom have obtained excellent positions. Several of our current graduate students obtained internships for this coming summer at government labs and in industry. We are also very happy that we are graduating our second undergraduate class which consists of 5 students, all of whom are either going on to graduate school or have obtained desirable positions. It is especially gratifying to me, as it is for the Department as a whole, that in the exit interviews I had with them, all those students expressed a very high level of satisfaction with our undergraduate program. The students also had some excellent suggestions for making the undergraduate program even better; this should prove to be very useful to the Department.

I look forward to the next few years and to being able to report about new developments in the Department and about the successes of our students, postdocs, and faculty.

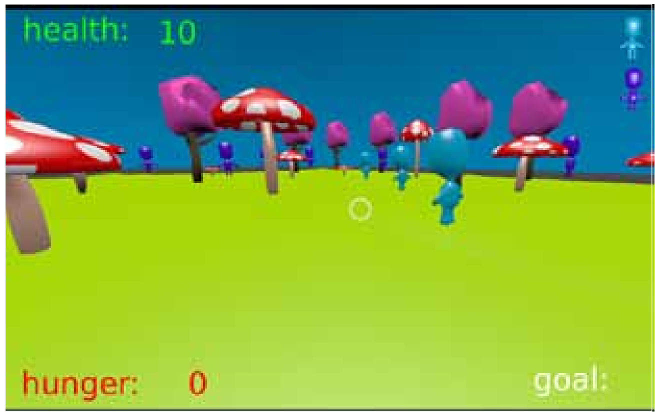
*Erlebacher, continued from Page 1*

different grid resolutions, Erlebacher and his collaborators implemented the RBF-FD in parallel over multiple CPUs and accomplished the first known implementation of accelerated RBF-FD on multiple GPUs. The implementation has strong scalability and significant speed-up, ranging from 2x – 9x depending on the size of the stencil or local region. During implementation, the problem geometry is partitioned and distributed across multiple CPUs, with common nodes of overlapping partitions synchronized by MPI communication. In addition, derivative approximations and explicit time-stepping are further parallelized on concurrent GPU hardware, with one GPU supplementing each CPU involved in computation. We expect additional acceleration through further GPU optimization.

"I like to develop algorithms on these GPUs – single GPUs and clusters of GPUs. When you solve very, very large problems, many numerical methods can become prohibitively expensive in terms of computing time. By using the GPU and these techniques, you can run more problems per unit of time or you can solve larger problems in the same amount of time. Those are the two main advantages. You know, many times when you do things, you like to get immediate feedback. So scientists may run large problems and it may take a month to get the results. But if you ran them on the GPU instead of taking a month, you maybe, might get it back in a day or two. In a day or two, you can produce an animation or something else, and look at the results. You can find errors faster, and you can do more studies."

Erlebacher began his career in research, accepting positions at NASA Langley Research Center and the Institute for Computer Science Applications in Science and Engineering in Hampton, VA after completing his Ph.D. in plasma physics at Columbia University. He arrived at FSU in 1996, and has been a champion of and contributor to Scientific Computing since its inception. Just as he began with a diverse research agenda, his scholarship continues to be diverse by its very nature. “I don’t have a research program the way other people have a research program. I tend to go from topic to topic, since I’m at the intersection of many fields. My interest in game design is one of those fields that intersects many different areas.”

Early in the process of thinking about games and game design, Erlebacher wanted to harness the power gaming could have to capture and hold students’ attention. Multimedia, voice narration, and player/audience interaction can be much more effective for learning than text and straight lecture alone. These varying modalities allow students and their decisions to trigger cause and effect in a virtual learning environment, seeing first hand the effects of their own actions. His effort has been very successful, and students from Political Science, Studio Art, Computer Science, Industrial Systems, Engineering, Music, Media production, Philosophy, Economics, Communication Biology, Physics, Mathematics, and Graphic Design have enrolled in the course.




Left: Image from Chomp Chomp, Yum Yum, a project from this Spring’s Game Design course. Chomp Chomp, Yum Yum was one of the entries in *Digitech 2013*, the university’s showcase of technology innovation.
Below: Erlebacher, Brandon Johnson and Nathan Crock discuss their research findings in the Visualization Laboratory.

“When I started the game design course, I was interested in games and their ability to facilitate learning or in helping develop or create educational games. Online learning is increasing, and will continue to increase because it gives more people a chance to actually get exposure to almost any subject you can think of. There’s been a drive over the last years with people talking about how to merge games with education. I mean, if you know people are playing games, and you know that your objective is to improve their knowledge or improve their education, somehow you gotta be able to join the two.”

Erlebacher’s most recent efforts are moving in that direction with the merger of games and education. He is working with the Department of Education to create a game where elementary and junior high students - kids ranging in age from 8 to 13 - would learn basic concepts of math such as fractions, proportions, equations, arithmetic, through a game. The object of the game is to have students who use the game reconstruct a city devastated by an earthquake. The concept is to allow the students to construct houses in various ways and through the construction, learn how to do certain types of optimizations – for instance how to construct a wall with a particular material while minimizing cost and maintaining a certain structural integrity.

“The student player is assigned various tasks that are solved through imagery, all the while receiving feedback as to progress. The idea is that to complete the game, students must master certain mathematical concepts - they’re learning math without the knowledge that this is the objective of the game. So in a sense, the education process operates in stealth mode. You’ve got to give them something they like, and at the same time ensure improvement of the math skills. This gives us exposure to the departments outside the scientific area. I think that SC applies not only to the sciences, but increasingly to the non-sciences where computers and mathematics play an increasing role.”

For more information, go to sc.fsu.edu.

# Computational Xposition 2013

## This year's Computational Xposition was a great success, and the inclusion of undergrads, grads and postdocs added more depth and breadth to the event.

Scientific Computing recently hosted the annual Computational Xposition, the department's research symposium for the academic year. This year's Xpo featured research from the largest number and widest variety of contributors in its nine-year history. Since 2004, the Xpo has been the venue to display the culmination of the year's research efforts and accomplishments. of graduate students; this year, however, was unprecedented, with poster submissions by five undergraduate students, eighteen masters and doctoral students, and four postdoctoral research associates. University Provost Garnett Stokes was in attendance at the event, and commented on the extensive range and impressive quality of the poster submissions. Research topics included epidemic networks, recording using multiple Kinects, groundwater hydrology for nitrate contamination analysis, image segmentation, and advection-diffusion equation methodology.

WEB EXTRA: Visit sc.fsu.edu/xpos for a retrospective feature of Xpo posters.

FACEBOOK EXTRA: You'll find more Xpo photos at https://www.facebook.com/FSUSciComp.

Clockwise from Left:(1) Doctoral student Arsia Takeh explains his poster, *Uncertainty Analysis of Inferring CCD using Crystaf*. Takeh's research examines the chemical composition distribution of copolymers and their mechanical and thermal properties. (2) Hans-Werner vanWyk points to a formula in his research, *Multilevel Quadrature methods for Stochastic Simulations*. Hans is a Postdoctoral Resesarch Associate. (3) Undergraduate students Ryan Learn and Ian Lozano review Ryan's resesarch entitled, *Numerical Studies of Penetrative Convection in Self-Magnetized Plasmas*. (4) Ph.D. student Rui Gu discusses the specifics of his poster, *Investigating Vesical-Substrate Interaction Using Two Phase Field Functions*.

# Steward accepts Post-doc at UCLA JIFREESE

After completing requirements for the Ph.D. in Spring 2012, Scientific Computing alum Jeffrey Steward accepted a position as Postdoctoral Research Fellow at the UCLA Joint Institute for Regional Earth System Science and Engineering (JIFRESSE). JIFRESSE is a scientific collaboration that was established to improve understanding and to develop future projections about global climate change and its effect on regional climates and environments. In conjunction with his post-doc appointment, Steward is a contractor at the NASA Jet Propulsion Laboratory (JPL) in Pasadena. JPL constructs and operates robotic planetary spacecraft, conducts Earth-orbit and astronomy missions, and operates NASA's Deep Space Network. Steward found out about his current post-doc through a combination of networking and old fashioned leg work.

"I found out about the JIFRESSE position simultaneously from two different sources. I actually first saw the posting on a mailing list for the Weather Research and Forecasting (WRF) model, which is the model I used for some of my graduate research. I also heard about the position very shortly after through a network of professors at Florida State who thought it would be a good position for me. It turned out to indeed be a perfect fit, so I am in debt to those FSU professors who had contacts at JPL through their research," said Steward.

While at the department, Steward studied many different mathematical tools, including Finite Element Method (FEM), optimization methods, partial differential equations, and fluid dynamics. He also took courses both in and outside SC that helped him acquire applied and analytical research skills appropriate for many different types of employment.

> "I found out about the JIFRESSE position simultaneously from two different sources.....It turned out to indeed be a perfect fit...."

"At DSC, I was able to study a broad variety of subjects and come in contact with a lot of different kinds of science. This is very important because while my area of emphasis for the degree was Atmospheric Science, I also learned computational and mathematical tools that were applicable to any kind of fluid, whether that fluid is the air going around the wing of a jet engine or the water, ocean and air of a raging hurricane. I ended up accepting a job improving hurricane prediction using satellite observations, which believe

Jeff Steward, Ph.D.

it or not is actually pretty similar computationally to improving the design of an airplane wing!"

"My interactions with my thesis advisor I. M. Navon throughout the program were invaluable. I cannot over-emphasize how much his direction in matters academic as well as professional were beneficial to me. I learned the invaluable tools and techniques of numerical optimization, data assimilation, optimal control, and adjoint development. His outlook on life and research were also instrumental in preparing me for my position. Through my interactions with Max Gunzburger I learned so much about mathematics, fluid dynamics, and how to give a great presentation. I feel very fortunate to have had the opportunity to read Max's books and have conversations with him. His multi-disciplinary approach to science is truly inspiring. My classes from Janet Peterson were also wonderful, and from her I learned the Finite Element Method and computational approaches to Partial Differential Equations. I also learned a lot from Gordon Erlebacher in my core courses regarding visualization and mathematical physics." Steward's coursework included classes outside the department that proved to be essential, especially those he took with Guosheng Liu in Meteorology, who has developed algorithms to retrieve cloud liquid water, cloud ice water, precipitation and surface turbulent fluxes using a combination of visible, infrared and microwave satellite observations.

At graduation, the position at JIFREESE was one of several job offers Steward received. "I had two offers and opportunities to work

*See Steward, page 8*

# Students prepare for summer, next phase

Serena Pham, Graduating Senior

Serena Pham will begin work at Oak Ridge National Laboratory in Oak Ridge, TN this summer on a three-month project. After the summer, Pham will transition to a long term assignment yet to be named. Pham's short term project begins in June, the main goal of which is to solve a set of 2 partial differential equations (PDEs) that describe a biomedical experiment in which vascular smooth muscle cells on one side of a porous filter migrate to the other side in response to a biochemical gradient. The biochemical gradient is described by a simple diffusion equation which is easy to solve numerically. The migration of the cells is described by a diffusion-advection equation which is not as easy to solve numerically. The cell diffusion term describes the movement of the cells due to Brownian motion and the advection term describes the movement of the cells due to the biochemical gradient. The purpose of solving these 2 equations is to find a value of the parameter in front of the advection term that will give results matching experimental data provided by the Vascular Research Lab at UT Graduate School of Medicine in Knoxville.

Pham is one of five graduating undergrads in the department this Spring. Other graduating seniors include Cameron Berkley, Brandon Johnson, Ryan Learn and Jerrison Li. Berkley, Johnson and Learn will return to DSC in the Fall to begin graduate studies.

## SC welcomes new Postdocs Zhao and Zhu

**Pengfei Zhao received degrees in mathematics from Jilin** University in northeast China in 2005, 2007 and 2010, with research interests in computational geophysics. He will work primarily on research involving methods of model order reduction implementing discrete empirical interpolation techniques on POD 4-D VAR trust region applied to fluid dynamics.
Pengfei and his wife Lei arrived in the U.S. in December, 2012. He works under the direction of Michael Navon.

**Born in northern China and raised in Shanghai, Ying Zhu** received undergraduate and graduate degrees in computational mathematics from Shanghai Normal University (SHNU). Afterward, he worked in the Department of Information Management of SHNU, teaching undergraduate courses in mathematics and programming, and doing research and evaluation of information service models. Ying's current research on image processing is supervised by Xiaoqiang Wang.
Ying and his wife Lichuan have a newborn son Yilai. During his leisure time, he enjoys classical music and reading, and making new friends at DSC.

Pengfei Zhao

Ying Zhu

Clockwise from left: Nathan Crock, Ben McLaughlin & David Witman.

## BEN MCLAUGHLIN

Doctoral student Ben McLaughlin was selected for an internship at Oak Ridge National Lab (ORNL) in Tennessee through ORNL's Higher Education Research Experience program (HERE). McLaughlin's mentor for the internship is Clayton Webster, whose research group works on a variety of projects including stochastic differential equations, model reduction, and uncertainty quantification. HERE is a program that provides research experiences for undergraduate and graduate students to enhance their academics. Applicants may identify research areas of interest across ORNL's breadth of research areas.

## DAVID WITMAN

This summer, Ph.D. student David Witman will intern at Pratt & Whitney, a company in East Hartford, Connecticut that designs and manufactures commercial and military grade gas-turbine (jet) engines. These engines power a wide range of aircraft from the sleek new F-35 Joint Strike Fighter to the Airbus A320 commercial passenger jets. "I will be working in the Hot Section Engineering department under the Advanced Methods group. The "hot" section refers to the majority of engine components aft of the combustor where temperatures commonly exceed the melting temperatures of the materials they are designed with. This means that precision in the design and testing process is an absolute necessity!"

Witman's research project will focus on pinpointing variation within the design and manufacturing process in to develop more robust and thorough analyses during the testing phase. "Completing this project will require a lot of the computational skills that I have learned during my time here in the department including stochastic processes and general algorithmic knowledge. Thankfully they are even giving me a day off to work on writing my thesis too!"

## NATHAN CROCK

From June 16 - July 27, Nathan Crock will teach in FSU's Young Scholars Program (YSP), a residential science and mathematics program for Florida high school students with significant potential for careers in the sciences, engineering, and health professions. Crock will teach a course he created entitled *Scientific Computing Essentials* three days a week in DSL 152. Since teaching the course last summer, Crock has refined the content of the lectures. The curriculum includes formal course work in mathematics, computer science, and science ethics for all students, as well as an elective course in molecular biology or modern physics. The emphasis throughout is on problem solving, integrating theory and application, and examining the ethical and societal framework of science and technology.

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The department's mission is to be the focal point of science and computation at Florida State University. Max Gunzburger is the Chair of the Department of Scientific Computing. He can be reached at 850.644.7024. Newsletters are issued three times each year. Subscriptions and single copies are available by calling 850.644.0196. This publication is available in an alternative format on request.

*Steward, continued*

with Computational Fluid Dynamics (CFD) that seemed very exciting. Both involved improving computational CFD tools for optimal design constrained by fluid dynamics. An example of this would be finding the best shape of an airplane wing that would maximize lift and minimize drag, thus improving the performance of the airplane." In making the final selection, though, he had a particular desire and a keen first hand interest in studying hurricane prediction. "I felt that after living in Florida and experiencing the awesome destructive power of hurricanes first-hand, I could probably contribute more to society by helping operational centers give earlier lead-times for hurricanes, thus saving lives and reducing property damage."

Currently, Steward is working on several exciting projects, including models that predict hurricanes. "I am working on improving hurricane prediction using satellite observations. All bodies emit radiation: you, me, the sun, the earth, and even the atmosphere. This occurs at all spectrums, so as strange as it sounds, you and I even emit microwave radiation! Satellites looking down at the earth can measure the radiation that the earth and atmosphere emit that reaches the top of the atmosphere. As this radiation travels upward, it interacts with whatever is in its path in several ways. For microwave radiation one of the most important of these interactions is scattering whereby radiation is sent bouncing in multiple directions. This happens mostly with large cloud particles such as cloud ice or cloud rain. By measuring these signals over a hurricane, we can work backwards how much rain or ice is present in which locations. By feeding this information in to a hurricane model, we can improve the prediction of the track and intensity of storms which improves the accuracy and lead-time of forecasts. This in turn can save lives and reduce property damage."

Steward's eventual goal is to teach, but for now, he's landed in exactly the right place, fulfilling both his professional and personal desires. "It's customary to do a post-doc after graduation for a few years if you want to go into teaching at a University, and teaching is my eventual goal. That said, for a post-doc, this position is my dream come true. Working at JPL in beautiful California I have come in contact with many of the researchers who I cited as I was writing my dissertation. I'm also able to have immediate impact on moving the field forward in directions that I think are important. I really love California. Los Angeles is a great city despite the traffic and occasional smog. Having the mountains and oceans together in such close proximity is why California gets earthquakes, but it's also why it's so beautiful."

> "[At DSC] I learned the invaluable tools and techniques of numerical optimization, data assimilation, optimal control and adjoint development. "

To see a program Steward wrote on fractals while at the department, go to: http://people.sc.fsu.edu/~jls07c/fractals/wadasphere1280x1024.bmp