Department of Scientific Computing

Fall 2015

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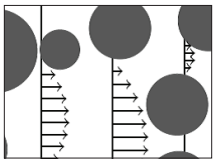

Time adaptivity for deformable capsules

A continued and unprecedented demand for interdisciplinary problem solving, especially in the realm of applied science, has fostered an alliance between science practitioners and mathematicians. Applied mathematician and SC assistant professor Bryan Quaife and his research play a critical role in that interdisciplinary alliance; his research program studies how mathematics can bring efficiencies to current estimation tools.

Bryan Quaife

"One of the tools I've been developing lately involves simulating deformable capsules submerged in a viscous fluid. These capsules are constantly changing -- they deform around each other, pass through constrictions, and develop and smooth regions of high curvature. As these simulations are advanced through time, the dynamics may become very complicated. To address this complexity, what one should do is take small time step sizes; otherwise the method might break or become unstable or an interesting phenomenon may be completely missed.

"On the other hand, if the capsules are far apart from one another, and their shape does not have regions with high curvature, then the dynamics become quite simple and one can start taking larger time step sizes. I've been developing algorithms that adjust the time step size based on the complexity of the dynamics; it's called "time adaptivity". The algorithm adjusts the time step size based on whether something complicated or something simple is happening. Moreover, it is fully automated so that a user does have to monitor the code to make sure that the method remains stable, and no trial and error procedure is necessary to ensure that an appropriate time step size is being used. In a paper that was just accepted in the Journal of Computational Physics, my co-author and I developed time adaptive algorithms for vesicles, a particular capsule that is used as a proxy for red blood cells in a capillary flow. These algorithms can be extended to a variety of other problems where the dynamics both complicate and simplify during the simulation. In such simulations, time adaptivity will be a useful tool for practitioners, engineers, and physicists."

Mathematics has always been fascinating to Quaife; he likes the way mathematics helps dissect, interpret, explain and predict behavior in complex systems. Quaife comes to Scientific Computing after spending four years as a Research Scholar at the University of Texas at Austin's Institute for Com-

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Alumni visits SC from national laboratory

Things have been good for Geoff Womeldorff since he completed his computational science Ph.D. in 2011. Following graduation, Womeldorff accepted a post doc at Los Alamos National Laboratory (LANL), a US Department of Energy national laboratory in Los Alamos, New Mexico.

"I went to Los Alamos in 2009 and met the person who would later become my wife -- so I was very excited to land a postdoc there. I love living in Los Alamos. It's a tiny little town on top of mesas, so there's nothing to develop and no sprawl. The average educational level is probably high above the norm."

One of the largest science and technology institutions in the world, LANL was founded during World War II to coordinate research and development of the Manhattan Project. Since then, the lab has been the birthplace of many variants of nuclear weapons, including the hydrogen bomb. Today, the lab performs a scientifically diverse set of interdisciplinary research in cancer, flow cytometry, national security and defense, magnetic fields, physics, biology, bioengineering, chemistry, and biochemistry.

GEOFF WOMELDORFF

"The lab is very interdisciplinary; traditionally you would say that Los Alamos is a physics laboratory. That's generally the thing that fits with their core values the most – prowess in physics. In the 40s and 50s that's where the lab started. My group, though, works to push scientific computing ideas, and we're starting to be successful in getting in the lead with projects. Lots of times people who work in the main science applications will feel like SC people are

Quaife, from Page 1

putational Engineering and Sciences (ICES). Originally from Canada, Quaife holds a Master of Science in applied mathematics from the University of Calgary and the Ph.D. from Simon Fraser University in applied and computational mathematics. His ideas for applied efficiencies across science disciplines lead to broad improvements by making connections between the different subject areas.

"Suppose that a practitioner is performing a simulation and is willing to accept a one percent error at the time horizon. A procedure that most people go through is trial and error -- they make a guess for a time step that will be used for the entire simulation and run the simulation in hopes that the one percent tolerance will be achieved. Assuming that the simulation completes, the error at the time horizon is computed, and if it's less than the tolerance, then they're satisfied with the results. However, if the error exceeds the tolerance, then this simulation is completely discarded and a new simulation with a smaller time step size is computed. People do this trial and error procedure multiple times to obtain a single simulation that they want for their particular application. With the time adaptivity methods that I'm developing, the one percent desired tolerance is dialed into the method at the start of the simulation, and time adaptivity will automatically commit the correct amount of error at each time step. In this

telling them how to do something better, but we need to figure out how to speak each other's language so we can help them design better systems and codes from the start instead of coming to fix something later. Something that we try to promote is this idea of using computer abstraction layer, code runtime or api to separate concerns."

LANL designs and builds some of the world's most advanced computing equipment for its research. It was home to the world's first supercomputer to achieve a petaflop of sustained performance, and the first computer accelerator/coprocessor or hybrid computer, which used dual-core Opterons to handle all the basic input/output, and a power cell processor attached to each Opteron core. Before securing a full-time permanent position, Womeldorff did an internship there, working on two ocean circulation models in the Climate, Ocean and Sea Ice Modeling Group. Being in this environment proved ideal for him, and in some ways mirrors his experience at Scientific Computing.

"At Los Alamos, we work a 9-80 schedule, so nine hours a day, five days one week, then the next week is three nine-hour days and one eight-hour day. So we have every other Friday off -- that's actually really nice. Something I definitely enjoy is the team atmosphere. Imagine a department that's like this but a hundred times bigger - that's sort of what being there is like. It's usually the case that if you have a problem, and you want to ask an expert about it, you can just say to them, 'Hey, can I come to your office and talk to you?' You generally have access to people and their expertise.

"I was part of a two-person team that was solving a problem over the last year – we were doing an experiment. Most days I would check in with my teammate and then once a week we'd have a meeting with our boss. My two-person team definitely felt like a team and when you add the person who was nominally the research supervisor, then that still feels like a team. Within our group we have a lot of line management structure and informality. It feels very collegiate – you can walk in people's offices and talk about their projects and sometimes they'll come ask you about yours. It's easy to get pure feedback as you progress through.

"I am grateful for the situation I'm in, so I wanted to try and share this career opportunity with people who are where I was when I was here. Sort of let them know here's what this life is like in the research lab I'm working in. I feel like the training that I got at this department was perfectly suited for the position I have now. The more you know about something, the more time you have to spend teaching, guiding and mentoring others. This visit is me getting started trying to contribute to the next wave of scientists. I love it. Never does a day go by that I don't count my blessings."

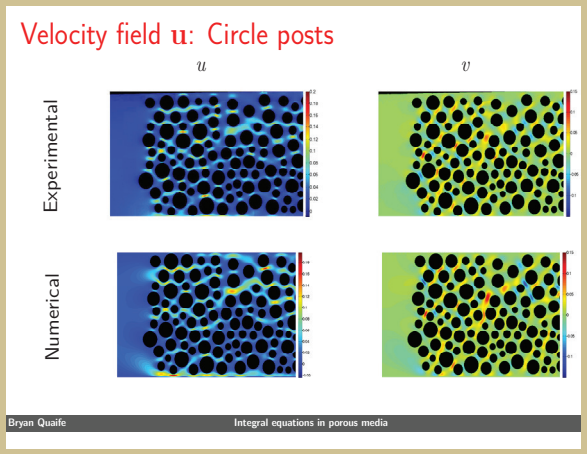
For more information on LANL, go to http://lanl.gov.

manner, the first and only simulation that is run is guaranteed to have an error close to, but less than, the desired tolerance."

For more information on Quaife, go to http://people.sc.fsu.edu/~bquaife/.

To find more about Quaife's Spring 2016 course on integral equation methods, go to http://people.sc.fsu.edu/~bquaife/IE-poster.pdf.

Right: A portion of Quaife's research entitled, *An integral equation method for flow in porus media*



SC welcomes new staff, postdocs & grad students

DAVID AMWAKE recently joined Scientific Computing's administrative staff as Administrative Specialist, and will handle grants and budgets. An FSU alum who graduated in 2007, Amwake holds dual degrees in human resources and business management. Before coming to Scientific Computing, he worked at FSU in Human Resources as an HR Specialist. In this position, his main duties involved assisting non-U.S. faculty, staff and graduate students -- primarily Research Assistants, Teaching Assistants, and Postdocs -- with employment appointments.

Although Amwake has lived his entire life in the South, his lineage is Italian, Canadian and American. He is especially close to his grandparents, from whom he learned the joys of Italian food. Amwake is married to Maribel, and is the father of two girls, Anabel and Isabel. When they have free time, he and Maribel like to do things with the girls, such as swimming, picnics, boating and other outdoor activities. He has an extensive collection of games that he plays on his pc, PlayStation 3 and Wii, and he likes reading fantasy and science fiction books (think Lord of the Rings). His absolute favorite is The Wheel of Time.

BRIAN BARTOLDSON was born in New York City and grew up in the suburbs of Dallas and Philadelphia. He earned a bachelor's degree in economics at Gettysburg College in Pennsylvania, and a master's degree in economics at FSU. Between earning those degrees, he volunteered for a year through AmeriCorps, which entailed living at the poverty line while working on community development projects.

After completing his masters program, Bartoldson worked at Charles River Associates, an economics consultancy headquartered in Boston, MA. After three years of programming and statistical analysis, he returned to FSU as a Scientific Computing graduate student. His interests in machine learning, statistics, math, science, and programming attracted him to the department, where he has been working with Gordon Erlebacher's Computational Neuroscience group. When Bartoldson isn't studying or working (he still consults part-time) he enjoys basketball, jogging, board and video games, popular math/science books, dancing with his girlfriend, and building sandcastles.

AMADO CRUZ has enjoyed living in Tallahassee since moving from Orlando in July to accept a Systems Administrator position at Scientific Computing. Before coming to FSU, Cruz worked as a Network Administrator for UCP of Central Florida. UCP is a charter school that also provides therapy services to special needs children throughout Central Florida. Cruz found the work especially rewarding, as he was able to help the people who devoted their careers to improving the lives of children with disabilities. He was previously employed at the Test Center for FDN Communications (now Windstream, Inc.) and in the NOC (Network Operations Center) for Cleartel (now Birch Communications) in South Florida. Cruz holds a degree in accounting from Nova Southeastern University, and an MBA from the University of Miami. When he's not at work, he goes outside to enjoy the weather. Often, he visits Tallahassee's parks and trails and enjoys reading poetry and watching Shakespeare's plays. One of the things Cruz enjoys about his new position is Wednesday Tea Time and getting a chance to talk with the next generation of people who will be involved in developing breakthrough discoveries in science and technology.

Postdoctoral associate LINDLEY GRAHAM grew up in the San Francisco Bay area, and joined the Department of Scientific Computing in late September to work with Max Gunzburger as a postdoctoral associate. Graham is a recent doctoral graduate, taking the Ph.D. from the University of Texas at Austin in Computational Science, Engineering and Mathematics. He received his undergraduate degree from the Massachusetts Institute of Technology in Aerospace Engineering. Graham studied coastal ocean modeling at UTA, and is currently working on research that focuses on parameter estimation for ice sheets and multi-fidelity Monte Carlo estimation.

Graham is a long time fencer, and has been fencing recreationally for over a decade. He is also an avid reader and enjoys board games.

MARIO HARPER enjoys dual U.S./Japanese citizenship, and is originally from Kyoto, Japan. He received dual undergrad degrees in Mathematical Physics and Economics from Utah State University, then contin-

ued his studies at USU to obtain a Master's degree in Finance. While at USU, Harper studied high speed convergence of stock market pricing algorithms, and did some work in modeling parasite dispersal. For a few years, he worked as a software developer and was the manager of a small ($10 million) investment portfolio for a local bank.

Harper chose FSU to pursue his Ph.D. because his research interests lie in visualization, virtualization and machine learning. He would like to use tools such as the Oculus Rift to control drone aircraft, and research ways to help machines learn quickly about their surroundings, then execute rational decisions without human input. This research has applications in fields ranging from autonomous submarines to automatic teller machines. Currently, Harper is enjoying all of his classes, but has a special interest in Sachin Shanbhag's course on Markov Chain Monte Carlo methods.

One of Harper's first loves is music; he chose opera and piano as undergraduate majors before switching to the sciences. He spends most of his free time with his wife Michaela and his daughters Mei (2 years) and Miyuki (3 months). He also likes to scuba dive (particularly shark and large animal dives) and cook.

IGNACIO ALVAREZ ILLAN comes to SC from the Universidad de Granada to work with Anke Meyer-Baese on improving diagnosis and prognosis of breast cancer. Recently, Meyer-Baese and Alvarez Illan received a coveted and prestigious award from the European Union's Horizon 2020 Research and Innovation Framework Programme under its Global Fellowships category to carry out this cutting edge cancer research.

Born in Madrid, Spain, Alvarez studied theoretical physics, then moved to Granada for his doctoral work in biomedical signal processing, focusing his research in computer aided diagnosis systems for diagnosis of dementia, such as Alzheimer's disease or Parkinson's disease.

Alvarez's techniques include the application of artificial intelligence tools for identifying patterns in medical images that correspond to brain impairment due to dementia. The algorithms he developed are able to learn significant features from images and classify new images according to the acquired knowledge. These tools are intended to aid and support physicians in difficult diagnoses and, in some sense, they are equivalent to having a very experienced physician on the team who has developed a sixth sense for diagnosis resulting from decades of practice.

The Universidad de Granada is one of the best universities in Spain, playing a major role in scientific output. It ranks as one of the world's best universities in many fields, including computing and mathematics.

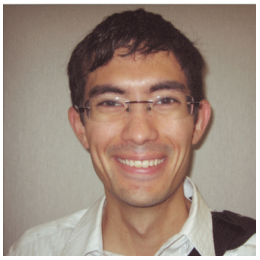
MARK LAMBERT, an SC masters student, joined the department this fall, having received the Bachelor of Science Degree in Biophysics from State University of New York at Geneseo in May 2011. Lambert is proficient in several programming languages, including C, Java and R. He


David Amwake


Brian Bartoldson


Amado Cruz

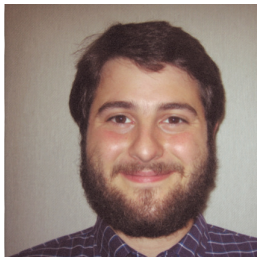

Lindley Graham


Mario Harper

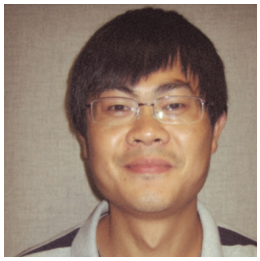
New additions to the department

Ignacio Alvarez Illan

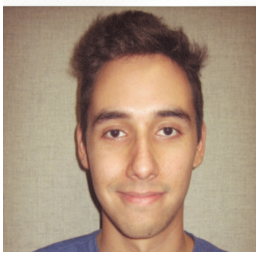
Mark Lambert



Eitan Lees



Hongzhuan Lei



Juan Llanos

has worked as a private tutor for college and high school students in mathematics, the sciences, and standardized test preparation, including the GRE. In addition to his private tutoring, Lambert began working as a tutorial assistant for Student Athlete Academic Services at FSU in Fall 2013, tutoring in math, biology, chemistry and physics; he has been employed with the Princeton Review to teach GRE prep classes.

Lambert was introduced to computational science in one of his classes, stating, [in one of my classes] "I was assigned a short rotation project to use Monte Carlo methods to fold a protein sequence and compare it to a known structure in the Protein Database (PDB) in the language C. During this project, I got my first real taste of computational science, and I would very much like to do more."

Originally from Chapel Hill, North Carolina, EITAN LEES received a bachelor of science in Physics from Appalachian State University in 2013. While in Boone, Lees did research with Brad Conrad on the fabrication and characterization of organic solar cells. Lees moved northwest to Ohio to continue his studies at Miami University of Ohio. He worked with James Clements and did research which focused on theoretical quantum optics, specifically collective quantum jumps of Rydberg atoms. Lees was awarded a masters degree in Physics in 2015.

Lees has many hobbies including juggling, improvisation, and badminton. He is looking forward to spending the next few years at FSU.

HONGZHUAN LEI is originally from the city of Shangrao, located in Jiangsu Province in southeastern China. He received his undergraduate and masters degrees from China University of Mining and Technology in Beijing, where he majored in Information and Computational Science and Geological Engineering, respectively. As a student, Lei was a recipient of the CUMT outstanding student scholarship and was awarded first place in mathematical modeling while a student.

After completing his masters in 2012, Lei worked for three years as a software designer at GoldenSun Petroleum Technologies in Beijing. While at Scientific Computing, Lei plans to work with Ming Ye on projects and research concerning groundwater modeling and simulation. His goal is to become proficient in using groundwater modeling, numerical simulation, and mathematics to study problems in engineering.

Lei enjoys fishing and exercising in his leisure time.

When JUAN LLANOS took Gordon Erlebacher's game design course as a computational science undergraduate student, he immediately wanted to know more, so he began a two-term directed individual study with Erlebacher, helping to design two educational video games – one of which helped teach basic arithmetic skills, the second, a philosophy game, taught ethical theory. With this first taste of research, Llanos was hooked on the challenges and rigor of problem solving, and began conducting a study with human participants. Llanos enjoys taking the math he learns and

applying it at the earliest possible juncture in programming classes, game design, and algorithmic problem solving.

Since the fall of 2014, he has been developing a simulation that studies neural networks through the use of the Oculus Rift virtual reality headset, and the Leap Motion 3D controller.

Originally from Colombia, Llanos is married to Debra Aly, and enjoys chess, reading, swimming, and playing and creating video games.

IAN MCCANN came to Tallahassee from Boca Raton, FL to study at FSU; he received a dual degree in Physics and Applied Math, graduating Spring 2014. During his undergraduate study, McCann worked with Ingo Wiedenhover in the nuclear physics department doing research on specific isotopes of nuclei in stars that were related to supernovas. Currently McCann is interested in computational neuroscience, the research in Gordon Erlebacher's group. He works at CARE, a campus program for first generation students, as a math and science tutor. There he mentors students and is available to all students who need help in math and science

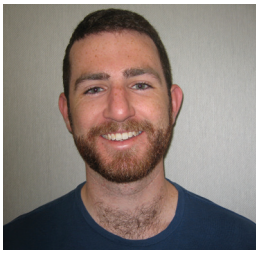
McCann spends his weekends going out with friends and playing sports.

Scientific Computing welcomes SERENA PHAM back to the department for graduate studies. In 2013, Pham was one of the first students to graduate from the computational science undergraduate program. In the interim years, she was employed as a researcher at Oak Ridge National Laboratory – where she worked on modeling biological factors in heart disease, web applications to handle biological data, and visualization for the Spallation Neutron Source. Pham was born and raised in Orlando, FL, and enjoys dancing Lindy hop, Balboa, and Blues. For her doctoral studies, her research interests are in numerical methods; currently she is exploring environmental applications - specifically geochemistry - with Ming Ye.

ALEX TOWNSEND knew all about Scientific Computing before enrolling as a graduate student, as he double majored in Computational Science and Environmental Science as an FSU undergrad. Townsend began working with Dennis Slice during his junior and senior years as an undergraduate student. He is from Saint Augustine in northeast Florida, the oldest city in the contiguous United States.

Townsend's research with Slice has focused on computational methods for modeling geographic variation of animal vocalizations. The studies center on how animal vocalizations vary across the geographic range of a species. By working with geospatial statistical and signal processing methods, Townsend has worked to computationally find spatial patterns in animal vocalizations. While still engaged in this research, Townsend hopes to branch out to more morphometrics-related work and more biomedically-focused applications of computational science.

In his free time, he enjoys many dif-

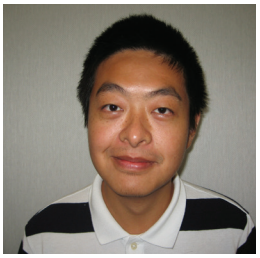


Ian McCann

Serena Pham

Amirhessam Tahmassebi

Alex Townsend



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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.

New to Scientific Computing, continued from page 7

ferent types of activities, including kayaking, hiking, sailing, golf, and video games. He also enjoys learning foreign languages and reading about ancient history and linguistics.

Originally from east central China, CHAOLUN WANG attended university in his home town of Wuhan at Wuhan University. After he was awarded the bachelor of science degree in biological science, Wang worked in Beijing for one year as a technician, helping a lab to analyze map-based cloning data. Although he enjoyed that position, Wang wanted to pursue the Ph.D., and emigrated to the U.S. to attend Florida State.

Wang's earlier research was in molecular biology and data mining, but on discovering his strength and interest in programming, he decided to pursue a computational science degree, preferring computational work to that of a wet lab.

Wang enjoys the outdoors; he hikes, camps and goes fishing every couple of weeks. He also spends time reading, cooking, playing cards with friends and watching movies.

As a new postdoctoral research associate, HUANHUAN YANG joined Max Gunzburger's group in September. She is originally from Hubei, a province in south central China, where she attended Central China Normal University and obtained her B.S. degree in mathematics in June 2007. She then earned her M.S. degree in mathematics, taking the subject of complex analysis, from Chinese Academy of Sciences in June 2010. In August 2015, she completed her Ph.D. thesis in computational mathematics at Emory University in Atlanta, GA.

Yang's research interests include numerical PDEs, reduced order modeling, inverse problems, and HPC/parallel computing. The principal subjects of her Ph.D. research are parameter estimation and reduced order modeling in cardiac electrophysiology. In her postdoctoral research, she will work on uncertainty quantification and reduced order modeling with stochastic PDEs.

Huanhuan Yang

Yang enjoys dancing, academic reading, and watching movies.

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