Department of Scientific Computing

Fall 2013

CONTENTS

Modeling for prediction

Structuring problems with the use of uncertainty analysis, uncertainty quantification, or verification/validation is rooted in isolating, then quantifying events that could happen, when a researcher is unsure whether they will or not. The problem, as Scientific Computing Research Scientist John Burkardt sees things, is figuring out the right way to dissect, then approach the problem.

"Making very complicated mathematical models of things like a nuclear reactor, or an airplane or a submarine or a bridge – involves many, many pieces. Part of the research for these areas requires looking very closely at individual pieces of a complex instrument to understand its physical characteristics. How strong is a piece of metal, and how likely is it to bend by a certain amount? How long is an electrical connection likely to work before there's a 50% chance it will fail? These are the kinds of questions you might ask yourself when modeling a problem. What you're trying to do is organize your understanding of a problem where you don't have control over everything," said Burkardt.

According to Burkardt, uncertainty analysis can be epistemic, stemming from incomplete knowledge, or aleatoric, caused by random variability in the system. Epistemic uncertainty can be reduced by additional experimentation or improvements in measuring devices, while aleatoric uncertainty is inherent and irreducible, brought on by factors that cannot be predicted, such as turbulent fluctuations of a flow field around an airplane wing.

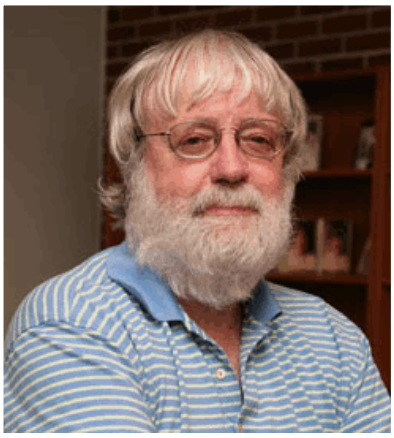
Burkardt uses this method to structure problems - to represent, characterize, and analyze the uncertainties in models. "Instead of saying, 'What is one plus two?' you're saying, 'What is the sum of one plus the amount of rain that's going to fall today?' I know it won't be a negative number, I know it's not going to be zero on this particular day, and it's probably not going to be 100 inches. You're doing the same kind of things you would normally do on the computer - adding two numbers - except now one of the numbers is not something you know, it's something that has a component of chance."

"If I had to make some other calculation, let's say I need to build a wall that's one inch plus the height of the rain in order to keep the rain from getting closer than one inch to top of the wall. The way I would answer that question would be to give you an answer that is on average right, or that 90 per cent of the time is right, or I can tell you an answer if you want 95% right. I can sort of build your confidence level assuming I understand how the rain works. And all we need is a 100 inch rain and I'm wrong. So that's the kind of thing you're doing in uncertainty analysis."

Burkardt thinks so highly of the method that he presents it in detail at scientific conferences like SIAM. Along with Clayton Webster at Oak Ridge National Laboratory, he has prepared a four-part presentation and workshop series and made it available publicly, so others who are interested can access and use it as desired. The technique allows him to focus on a portion of the

See Burkardt, Page 2

Message from the Chair



DSC CHAIR MAX GUNZBURGER

....[F]aculty are very well funded, are able to attract excellent students, collaborate with researchers all over the world, are invited to give talks at top international meetings, and hold leadership positions in professional societies.

This year, the faculty is focusing on an examination of our degree programs and courses with an eye to ascertaining if changes need to be made to better serve students. Of course, this effort is simply a concentrated version of what we have been doing since the inception of those programs. We continually respond to feedback we obtain, both solicited and unsolicited, from students; we have found such feedback to be an invalu able resource. Although we do not foresee the need for major changes, even some seemingly small changes, e.g., changing the order that courses are taken by students, additions and deletions to syllabi, etc., can have meaningful impact on student experience and learning.

At the same time that the faculty have engaged in this introspective examination, they, together with students and postdocs, continue their thriving research programs which, by every measure, are very successful. For a non-wet-lab department, the Department faculty are very well funded, are able to attract excellent students, collaborate with researchers all over the world, are invited to give talks at top international meetings, and hold leadership positions in professional societies. As we have done in the past, we will continue to feature the research of faculty in this newsletter.

This year marks a new cycle in the careers of our alumni who received their Ph.D. from our department. Our students have been extremely successful at obtaining postdoc positions at top laboratories and universities, so our success in initial job placement has been nothing short of great. Now, some of those are completing their postdocs and are looking for a second job, often of a more permanent nature. Early indications are that they are succeeding in this regard as well. We will report on this in future newsletters.

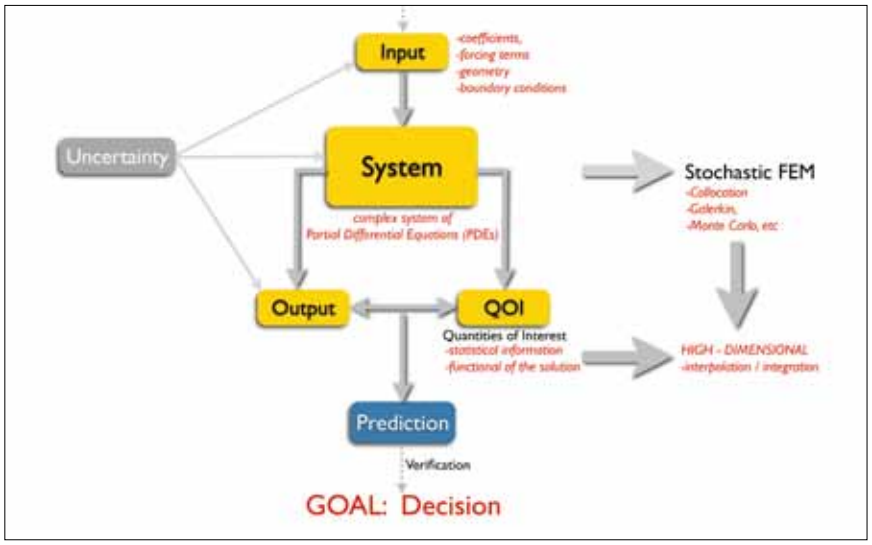
Burkardt, continued from Page 1

problem and determine how that particular piece contributes overall, an approach that is especially important where there is a possibility of threat to human life or when it relates to high dollar risk.

"As an example, if we build a nuclear reactor in this town, I can tell you right now there's a chance it will blow up. But the chance of this thing happening goes back to the situation that I know the range of things that can happen in a nuclear reactor, and if some things happen at the same time, then it will be a bad situation. But how often does that happen? So there again, you're looking for, in this landscape, where are the places where some quantity gets above some value? In this case, we might think of it as the temperature of the core of the nuclear reactor. If it gets too hot, we'll have to close up and move to Belgium. It comes down to calculating measuring and understanding the scope and scale of risk. How can I understand what the scale of risk is, given that there are risks people live with every day and accept, such as driving? Driving is something people never think about which represents the greatest risk of death that most people face, but we think nothing of getting in a car and driving wherever we want to go."

SOFTWARE RESEARCH

As an additional component of his work, Burkardt is sampling currently available software components to advance this type of complex research. By combining relevant and useful pieces of one or more software programs, Burkardt hopes to find a versatile program to use for research in teaching that will make it easier to execute the computations of interest.



From "Uncertainty Quantification Model from Analysis of SPDE's and Numerical Methods for UQ, Part I: Background, motivation, and tools of the trade", a tutorial presented at the SIAM Conference on Uncertainty Quantification, 03 April 2012, by Clayton Webster and John Burkardt.

"I've been trying to figure out a way of getting a good program to use. The problem right now is that if somebody wants to do an example program or a problem involving the study of a window or a wing, or anything like that, typically what you do is you start writing your own program and that takes a long time to do. It's a huge investment. So other people, instead of writing their own program, can just take someone else's program and use it. Even though they may not understand right away how it's set up, it's a big saving for them to spend the time to learn how that program is set up and use it rather than starting from scratch. They'll understand a program they wrote themselves, but it would take a long time to write."

Burkardt plans to use this software to advance research with finite element calculations, which help scholars study fluid flow and heat flow among other things. Studying what happens when there are forces on a shape such as the shape of a car or the shape of a wing requires a tremendous amount of information. "As you can imagine, describing the shape of a car is not easy. After you describe the shape, then you have to say how do I replace that shape by little teeny shapes? And how do I put extra teeny shapes near parts that I know are going to bend a lot? I need to have a lot of information in those places. And then after I've got my shape set up, then comes the hard part. Then you have to put these little sensors everywhere to gather information in order to assess what's happening. What am I doing here? What's happening in this spot? Is it getting bigger? Is it getting smaller? Am I pushing into my neighbor? And so on."

The software would be a valuable time saver for Burkardt and his faculty collaborators, but also for SC students. Once a student learns how to perform these techniques, doing them over and over again for each problem they work on is of limited value, as the tasks are time consuming and don't increase their knowledge. Burkardt is working to build a library of software programs or code that has already been written, and give users access to pieces they need for their individual projects. "If we can do that, we'd be able to mix and match in a way that is beneficial to any particular project. This would let us go through the steps very quickly so that what happens is we can all get to the important thing which is solving problems. You want to spend less time writing programs and more time doing numerical experiments."

"If we can do that, we'd be able to mix and match in a way that is beneficial to any particular project. This would let us go through the steps very quickly so that what happens is we can all get to the important thing which is solving problems. You want to spend less time writing programs and more time doing numerical experiments."

For more information, check out http://people.sc.fsu.edu/~jburkardt/.
If you look closely, you'll find some cool puzzles there, too.

New grad student accepts position at GM

When new grad student Brandon Johnson decided to attend the Fall 2013 Engineering Day, he planned to get acquainted with the recruitment process and prepare himself for a future job search. He surveyed the list of corporations who would be in attendance, looking exclusively for technology companies. When he arrived, he noticed that although General Motors wasn't on the list, GM representatives had a table and were interested in hiring graduates who either had backgrounds or majors in technology. Johnson decided to talk to them.

That conversation turned into a first interview, then another, and finally, a job offer. "I talked to the reps at Engineering Day, and they were impressed by my resume. After that, I interviewed by phone with General Motors headquarters staff in Detroit. Finally, they flew a guy in from Detroit specifically to interview me; a few weeks after that, they made me an offer."

Johnson thinks GM was impressed by a couple of key things. First, he believes they were impressed by how he manages his time. Second, he thinks the quality and scope of the research he did as a Scientific Computing undergraduate indicated his software fluency and demonstrated his ability to transfer those skills to practical use.

"I think they were impressed by the quality of research I've done and by my ability to manage my time. I graduated from the undergrad program in three years, and I played baseball at the same time. They were also very impressed by the point cloud recording research practicum I did using multiple kinects. In the project, I used two 3-D cameras at different angles to record the same object. Afterward, I placed the recordings on top of each other, giving viewers a 3-D recording of the entire room in which you can zoom in and out. This type of research has a lot of applications, from video games to hazardous materials usage. Really anything where simultaneous localization and mapping could be beneficial."

Johnson's future position will be based in Atlanta, and he's excited about that. "I'm looking forward to living in a big city, and it's nice to have a job waiting for me instead of the other way around. My purpose for joining the SC masters program was to learn more so I would be an attractive job candidate. I definitely like the freedoms and high academic expectations here in the department."

SC Grad Student Brandon Johnson

New grad students, postdocs & staff

WHITNEY BANKS is Scientific Computing's new Academic Support Assistant, and will take on the role as the new academic advisor for the department. Before coming to SC, she attended Tallahassee Community College. Banks is from South Florida, is a theatre enthusiast, and loves to perform and entertain. One of her recent roles was at Tallahassee Little Theatre in the play, A Christmas Carol. She loves to meet new people, and is looking forward to her new position.

JUSTIN BRICKER attended the University of Florida where he graduated in Spring 2013 with a Bachelor of Science degree in mathematics and a minor in chemistry and bioinformatics. While at UF, Bricker's research modeled the growth of apocnemidophorus pipitzi, a stem-boring weevil and its impact on the Brazilian Peppertree. He was involved in several bioinformatics research projects including the discovery of gut microflora related to the onset of Type 1 Diabetes in non-obese diabetic mice. Since arriving at Scientific Computing, he has been working with Peter Beerli in his laboratory.
Bricker spends his leisure time playing tennis and racquetball, biking, weightlifting, reading, watching movies, playing board games and tinkering with electronics. He is from Naples, Florida, and is pursing the Ph.D.

Originally from New York, masters student MICHAEL CONRY studied at the State University of New York at Purchase, and was awarded dual bachelor degrees in mathematics/computer science and new media in May 2003. While at SUNY Purchase, Conry received the Natural Sciences Award for Outstanding Service by a student. He also served as a teaching assistant for three years, helping teach web design, HTML, Javascript, databases for web applications in PHP, MySql and XML. Conry is co-author and editor of the textbook, Sustainability Manual. Conry studied jazz and bass, and in his very limited free time, plays music with friends, enjoys photography and reads novels. He is working with Alan Lemmon on genome sequencing research.

Doctoral student BENJAMIN CRYSUP earned two bachelor's degrees while studying 30 miles southeast of his home town of Bastrop, at the University of Texas at Austin: one in chemical engineering, the other in computer science. While at UT Austin, Crysup worked in a cancer research laboratory performing cellular biology experiments. His interests are broad, and include mathematics, polymer science, and computers.
When he isn't jogging in state parks or playing video games, Crysup spends his free time doing game development. For the last two years, he has been developing Ignis Spent, a multilevel video game which matches difficulty to the player and uses techniques from process engineering. The result is that the game challenges the user in a player-specific manner. Crysup plans to market the game and have it available for sale in two years.


Whitney Banks


Justin Bricker


Michael Conry


Ben Crysup

New grad students, postdocs & staff, cont.


Daniel Fratte


Brandon Johnson


Ryan Learn


Jason New

DANIEL FRATTE hails from Mendoza, a city in the north western region of Argentina, located on the eastern side of the Andes mountains. He studied software engineering at the Universidad Tecnológica Nacional where he was awarded the Bachelor of Science degree in Information Systems Engineering in December 2011. Fratte is a masters student, and was the recipient of the Argentine Presidential Fellowship in Science and Technology, and placed 3rd in the 5th Congress of Systems Engineering Students Best System Contest with his thesis. After graduation, he worked as a python and java programmer and .NET engineer with the Huddle Group. Fratte is interested in physics, climatology and astronomy, and plans to work with Tomasz Plewa studying computational astrophysics, a research topic that he finds fascinating.
Fratte is a biking and martial arts enthusiast, and enjoys reading and scientific research.

After BRANDON JOHNSON completed his undergraduate degree at SC in May 2013, he returned as a masters student to continue his studies. Johnson's advisor is Gordon Erlebacher, and as an undergrad, he did research on Point Cloud Registration using multiple Kinects, which he presented at the 2013 Computational Xposition. Johnson pitches for FSU, and represents the baseball team on the Student Athlete Advisory Council. He also attends Atlantic Coast Conference meetings on behalf of the university baseball team. Johnson is featured in a related story on page 4.

SC doctoral student RYAN LEARN was awarded an undergraduate degree in Scientific Computing last year, and has worked with Tomasz Plewa for the last year and a half, studying such varied phenomena as instabilities in laser-driven plasmas and stratified convection with stellar interiors. Learn is from Orange Park, Florida, a suburb of Jacksonville.
Learn spends much of his free time biking around town, and he enjoys flying kites when the weather cooperates. He also enjoys reading and is developing several hobby projects, such as network theory epidemiology models and beer recommendation programs based on Bayesian inference.

Doctoral student JASON NEW is from Port Saint Lucie, Florida, and recently completed his BS in Meteorology at FSU with a major in Applied Mathematics. While an undergrad, he studied the trajectories of air parcels at the extremities of fast-moving low pressure systems and wrote an object oriented C++ program which parsed through data files for a program called GrADS.
New has a multitude of companions at his place, including three cats, four mice, a Betta fish, a baby gecko and a bonsai tree. New teaches object oriented programming for the Program in Interdisciplinary Computing in addition to his coursework. When he claims a few minutes for himself, he relaxes with his fiancé or plays with his pets.

Doctoral student BIKASH SAHA is licensed as a Professional Engineer in Florida. Before joining Scientific Computing, he worked with URS Corporation in computational hydrodynamics, and was awarded undergrad and graduate degrees in civil engineering from Bangladesh University of Engineering and Technology and Tennessee Technical University, respectively.
Saha's research on deep sea geohazard modeling is directed by Ming Ye. Together, they are working to develop a robust numerical debris flow model that can analyze complex behavior of submarine debris and mud flows that pose threats to the deep sea transportation lines.
Saha likes to play tennis and soccer, and enjoys gardening and salt water fishing.

NICHOLAS SCHACHTER grew up in New York and Connecticut, and attended college at Hampshire College in Amherst, Massachusetts. Schachter

majored in applied mathematics with a specialization in algorithm design and implementation. While an undergrad student, Schachter interned at Smiths Detection Danbury, a company that makes chemical detection instruments for the TSA, the US Army, and various other groups. His prior research includes optimizing principal component analysis for noisy data, estimating the optimal dimensionality reduction for a data set, Tensor Factor Analysis, and investigating the possible use of combinatorial methods in data analysis. Schachter likes to play soccer and recently joined a local 6v6 league in an attempt to start playing more regularly again. He also enjoys reading fiction, playing/watching sports, and playing instruments (cello and keyboard). Schachter is pursuing his masters degree.

Originally from San Jose, California, masters student ARIA SMITH received a B.S. in Mathematics in May 2013 from Clark Atlanta University. At Clark Atlanta, she studied the application of Newton's Method in dynamical systems and spent a summer as an undergraduate researcher at the Naval Research Laboratory in Washington, D.C. where she developed a spectral detection algorithm for hazardous materials. Smith presented her first poster as a graduate student in December entitled, "Spectral Detection Algorithms for Photo-Thermal Imaging."
In her free time, Smith enjoys spending time with friends, watching both college and professional basketball and football games, and doing a little shopping. She also loves working with children and tutoring in mathematics.

For the next year, XIANKUI ZENG will work with Ming Ye as a postdoc to study groundwater modeling and uncertainty quantity quantification. The research will focus on groundwater protection and management in China. Zeng works at the Xianlin Campus of Nanjing University, a comprehensive research university in Jiangsu Province located on the coast in east central China.
He received his BS and MS degrees in 2007 and 2009, respectively, from Jilin University, where he studied Hydrology and Water Resources and Groundwater Science and Engineering. The primary focus of his research has been hydrologic frequency analysis, sensitivity analysis of groundwater modeling, and uncertainty analysis and assessment of groundwater numerical simulation.
Xiankui is single, likes sports - especially basketball – and is a big fan of the NBA. He would like to improve his conversational English while he is at Scientific Computing, and welcomes spontaneous chats with his SC colleagues.

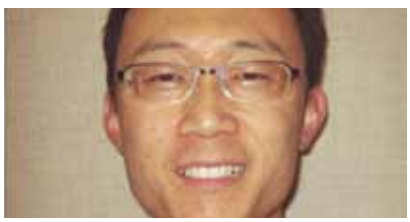
Doctoral student WENJU ZHAO is from Rizhao City in southeastern Shandong Province in China, and received his bachelor's and master's degrees in computational mathematics from Shandong Normal University and Jilin University. His research interests are in numerical solutions for partial differential equations and numerical analysis. His previous research centered on stochastic volterra integral equations, stochastic boundaries in scattering problems, and finite element approximations of Cahn-Hilliard-Cook equations. In addition, Zhao is fluent in several programming languages and computer scripts.
In his spare time, Zhao enjoys climbing, running and swimming. He plans to study hydrodynamic fluctuations in fluids with Max Gunzburger.


Bikash Saha


Nicholas Schachter


Aria Smith


Xianku Zeng


Wenju Zhao

Department of Scientific Computing
400 Dirac Science Library
P. O. Box 3064120
Tallahassee, FL 32306-4120
www.sc.fsu.edu

First Class
US Postage
PAID
Tallahassee FL
Permit 55

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.

Ashki leans in


Ph.D. Student Haleh Ashki

Inspired by Facebook executive Sheryl Sandberg's book and the Graduate Cohort Workshop, Haleh Ashki and a fellow student created a Lean In circle for FSU women in the computing sciences. Lean In circles foster career support and encourage professional advancement strategies for women. Currently, Ashki is preparing materials for the circle, and getting organized for the meetings. "I attended the Graduate Cohort Workshop, and was excited about the possibilities for collaboration between and among women in computational science, computer science and engineering. When I got back to Tallahassee, I decided to make a circle for women students in computational and computer science. I made the Lean In circle and named it Nole Girls. Now we're working on making the slides, gathering the information and getting everything ready for the meetings. We plan to start meeting in the Spring semester."

Ashki is promoting the circle across the campus in the sciences. She is excited about the possibilities the collaboration can bring. "We plan to have lots of good talks on how to survive in graduate school, how to study efficiently, how to manage your time, how to find a job, where to apply for internships, and many others. I can't wait to get together and share our experiences and strategies."

For more information or to join the Nole Girls circle Ashki created, go to leanin.org. For more on the Graduate Cohort Workshop, go to http://cra-w.org/. You can find info on Ashki's research at http://people.sc.fsu.edu/~pbeerli/Beerli_Lab/Student.html.

SC.FSU.EDU facebook twitter