Department of Scientific Computing

Summer 2010

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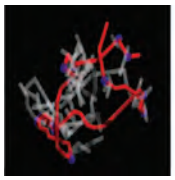

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Shanbhag receives NSF Early Career Award

Scientific Computing, established in 2009, has its very first faculty recipient of an NSF Early Career Award. Sachin Shanbhag, an Assistant Professor, received the prestigious award to continue his research on computational rheology of polymer melts. Unlike typical solids and liquids, "gooey" materials like polymer melts, foams, suspensions, and gels have both solid-like (elastic) and liquid-like (viscous) properties. Rheology is the study of how such viscoelastic materials respond to deformation.

This award is a second important award for Shanbhag; he also received the Petroleum Research Fund New Faculty Award in 2008. Shanbhag graduated in 2004 from the University of Michigan, Ann Arbor, with a degree in Chemical Engineering. After spending two years as a postdoctoral research associate at Michigan, Shanbhag accepted his current Assistant Professorship at Florida State.

"The career award recognizes the quality and impact of Dr. Shanbhag's research on polymers, tissue engineering, and nanotechnology applications and the even greater promise his work has for the future," said Max Gunzburger, Chair of the Department of Scientific Computing. "The timeliness and innovatory nature of Dr. Shanbhag's research also benefits students who, through the courses he teaches and the advice he provides, learn how to solve cutting-edge problems in important areas of engineering, scientific, and computational research."

Prior to his arrival at FSU, Shanbhag focused on developing rheological models for polymer melts. These mathematical models use information about the chemistry, branching structure, and composition to predict the viscous and elastic properties during deformation. A significant amount of progress has been made since then, and contemporary models have become both sophisticated and predictive.

Over the next five years, Shanbhag will focus his research efforts on doing the exact opposite by trying to infer the structure and composition of an unknown polymeric sample by using rheological data as input. This process of using computational models to infer what we cannot see, or measure directly, has been dubbed as "analytical rheology". The primary motivation for this undertaking is that unlike standard analytical techniques such as chromatography and spectroscopy, rheology is extraordinarily sensitive to molecular structure. His preliminary work on the problem, recently published in Rheol. Acta., has been hailed as an important breakthrough.

Shanbhag is excited by the possible enhancements his research can lead to in the training of students. He has been teaching courses for the College of Engineering and the Department of Scientific Computing and will use his award to focus his research and teaching on two specific areas. First, he plans to enhance minority involvement in his research. Second, Shanbhag will leverage computational methods to emphasize the connection between microscopic and macroscopic properties in coursework.

"Florida State University's close proximity and collaborations with Florida A&M University gives me a unique opportunity to expose minority students to research. Upwards of 50% of the students in the undergraduate classes I've taught in thermodynamics and chemical kinetics come from minority groups. So far, I've been successful at recruiting a couple of minority students every year, and the goal is to maintain that level, while encouraging some of them to take up research careers or go to graduate school."

Sachin Shanbhag

Max Gunzburger, DSC Chair

From the Chair

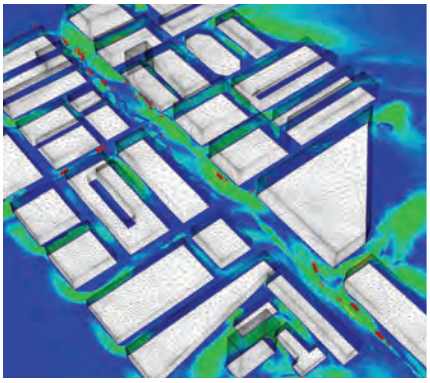
We had an eventful summer in the Department of Scientific Computing. We graduated the first student, Pablo Seleson, who completed our Ph.D. program in Computational Science. One of our junior faculty members, Sachin Shanbhag, was awarded the prestigious NSF Early Career Award. In addition, we put the final touches on the B.S. program we are launching this coming fall and, during orientation sessions, met up with the first group of students entering the program.

This newsletter features Pablo and Sachin (a future newsletter will feature the undergraduate degree program.) It also features the influential research program of one of our senior faculty members, Michael Navon. Thus, the newsletter manages to provide a glimpse at the "vertical" quality of the Department by featuring the research of a graduate student and of a junior and senior faculty member. We hope that in the not too distant future, we will also be able to feature the research of our undergraduate students!

Chair, Department of Scientific Computing

Professor Collaborates on Data Assimilation Research

Collaboration is the hallmark of Professor Michael Navon's research. For the last ten years, he has been associated with the Applied Modelling and Computation Group (AMCG) at the Imperial College of Science, Technology and Medicine in London. The AMCG concentrates its efforts in developing and applying innovative modeling techniques for earth, nuclear, engineering and biomedical sciences. AMCG has core research interests in numerical methods for ocean, atmosphere and climate systems, engineering fluids including multiphase flows, neutral particle radiation transport, coupled fluids-solids modeling with discrete element methods, turbulence modeling, inversion methods, imaging, and impact cratering. This summer and for the next two years, Navon travels to London to work on research that will apply data assimilation techniques used to study many topics – from nuclear reactors to coastal defense and flood forecasting. Navon and Imperial College professors will apply operational tools for the prediction of ocean/atmosphere behaviors, use uncertainty in engineering calculation and implement reduced modeling for rapid assessment.

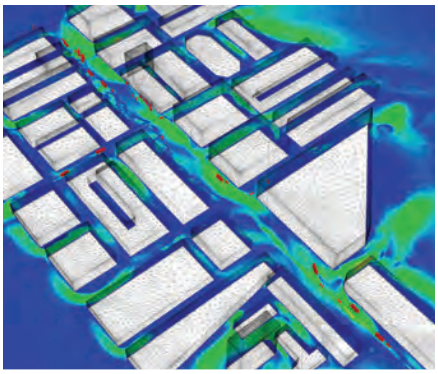


This most recent alliance is the result of Navon's assistance in helping AMCG obtain a large research grant from the Engineering and Physical Sciences Research Council (EPSRC), an international counterpart to the National Science Foundation. The grant they received will help them apply data assimilation techniques to study many topics – from nuclear reactors to coastal defense and flood forecasting. Navon and Imperial College professors will apply operational tools for the prediction of ocean/atmosphere behaviors, use uncertainty in engineering calculation and implement reduced modeling for rapid assessment of terrorist threats in a joint proposal to the military.

"I was invited to work with Christopher Pain, Fangxin Fang, Gerard Gorman, Matthew Piggott and Peter Allison, all of whom are doing exciting and cutting edge research in ocean modeling. They are incorporating some of my ideas and previous joint research in the 3-D adaptive mesh fluid model. We hope this will increase accurate prediction of free surface dominated flows in coastal regions."

Broad and comprehensive, Navon's research involves computational mathematics and geosciences research. His projects address expansive themes such as mathematical modeling of complex geosystems. Often, he works on several research projects in parallel.

Geoscientists and researchers study the earth's systems and its evolution in comparison to its current state. Geosciences encompass the study of many aspects of the earth, including geology and geological phenomena, geophysics, oceanography, and the atmosphere. Being part of a field that contributes to research that is important to understanding and preserving the earth's systems is exciting for Navon. "Research in the atmospheric, earth, and ocean sciences is only part of geosciences today. Geosciences research addresses the nation's need to understand, predict, and respond to environmental events and changes so as to use the Earth's resources wisely. We need to know more about our environment and resources such as water, energy, minerals, and our biological diversity."



The research Navon is undertaking with Imperial College has many practical applications, some of which are particularly germane to residents in a coastal state such as Florida. The model will help Navon and his collaborators advance methodologies that better predict the impact of disasters such as the one currently in progress, the Deep Horizon oil spill in the Gulf of Mexico. "The model will allow us to use wetting and drying methods to help us see how and where the tide flows and recedes from the beach. For instance, if you have the oil pollution in the Gulf, you have a beach and you want to find out how much oil is seeping into the sand. By using this type of simulation, we may be able to predict how much oil has penetrated into the sand. This process may take many months."

Left: (a) Urban geometry (b) Tracer distribution (traffic and boundary layer integration into the model; Low ambient wind; Multiple 300 minute experiments; 15 minute release of PFCs; Wind tunnel simulations (1/200))
Right: (a) Urban geometry (b) Tracer distribution (traffic and boundary layer integration into the model; Low ambient wind

First Student Completes Ph.D. Program

Pablo Seleson, Ph.D.

Multiscale Material Modeling

Computing

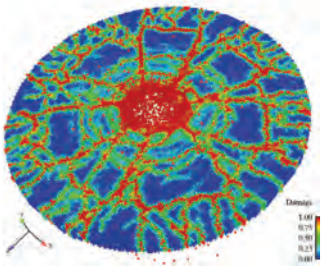
PERIDYNAMIC MODEL

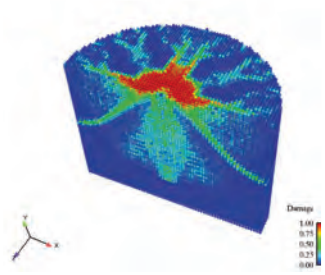
Nonlocal Formulation

Dispersion

Fracture PERIDYNAMIC MODEL Scientific Computing Ph.D.

With his studies in multiscale material modeling, Scientific Computing has its very first student complete its Ph.D. program in Pablo Seleson, who graduates in the Fall. Seleson successfully defended his dissertation entitled, "Peridynamic multiscale models for the mechanics of materials: constitutive relations, upscaling from atomistic systems, and interface problems" on July 20, 2010. Seleson's research centers on a continuum mechanics model called peridynamics, a nonlocal extension of solid mechanics. A distinguishing characteristic of peridynamics is that in contrast to classical mechanics, it has an integral formulation that allows users to describe fracture processes.



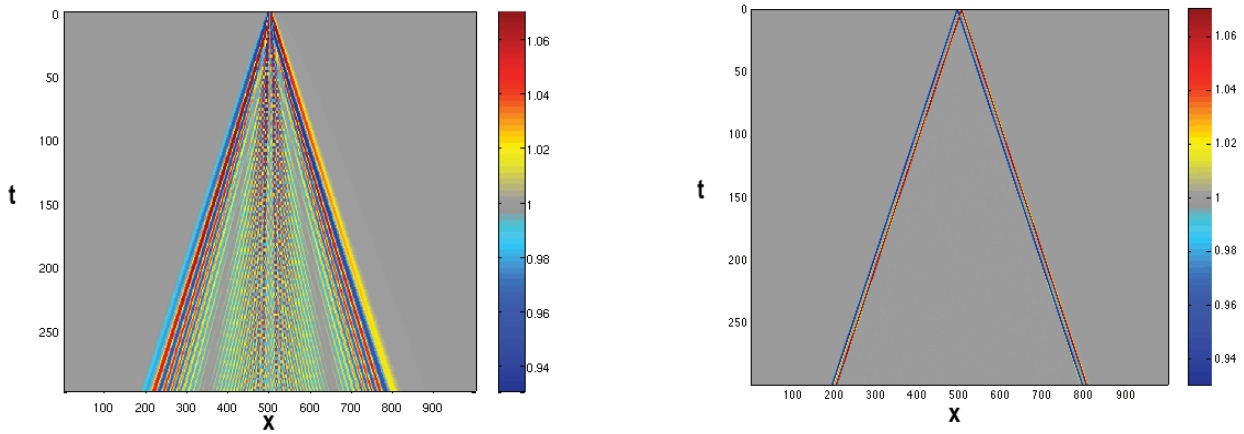


Figures a (left) & b (right): Peridynamics simulation using the PDLAMMPS code of the impact of a hard sphere on a brittle target; projectile hidden so as not to obscure target. The targets are colored by damage, with blue representing 0% damage, and red representing 100% damage. Note the emergence of a Hertzian crack in (b).

Seleson focused his research on the multiscale aspect of peridynamics. He connected peridynamics to atomistic systems and showed it is possible to derive continuous peridynamic models that preserve dispersion effects inherent to molecular dynamics models. He also showed the multiscale and multimodel capabilities of peridynamics by deriving a nonlocal formulation of interface problems. Seleson worked under the guidance of Max Gunzburger. "I had such a great opportunity working with Max. I received excellent guidance and wise advice from him. He allowed me to grow as an independent researcher, and I was able to work with some of his collaborators at Sandia National Laboratories and that has been an enriching experience."

Born in Argentina, Seleson attended Hebrew University of Jeruselem, studied physics, philosophy and cosmology and wrote his master's thesis on galaxy formation and dark matter. In 2006, Seleson came to Florida to the School of Computational Science. He recalls, "I was about to finish my master's degree in Physics and I was looking for opportunities to come to the U.S. to get a Ph.D. One particularly interesting option at the time was the School of Computational Science here at FSU. It offered a program where the courses, the facilities and the environment were all oriented to scientific computing."

Because of his experience in large-scale simulations in cosmology in Israel,

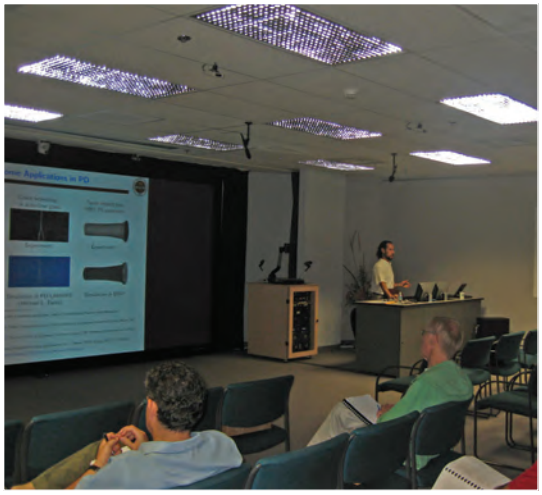


Figures a (Left) and b (Right): Density evolution of the propagation of a smooth initial pulse, comparing the nonlocal continuum peridynamics model (a) and the classical local wave equation model (b). Time is represented by the y-axis (from top to bottom), and the x-axis represents the reference configuration of the nodes in a one-dimensional system. The colors represent the density, and dispersion is numerically manifested as broadening of the lines. The nonlocal model (a) is more dispersive than the local model (b).

Seleson was persuaded by the possibility of continuing to work with computational simulations, including high performance computing. "I was working with computational simulations, and although I wasn't expecting to continue working in the same field, the computational tools are similar. One of the things you consider when you want a career is learning and working in a field you find interesting. But also you have to make sure you acquire good enough tools that will allow you to work in other fields as well."

Now that graduate school is behind him, Seleson has turned his thoughts to his next endeavor. In the Fall, Seleson and his wife, Esther, are moving to Austin, TX where he has accepted a prestigious ICES Postdoctoral Fellowship at the Institute of Computational Engineering and Sciences, located at the University of Texas at Austin. Seleson will work with J. Tinsley Oden and Serge Prudhomme, two leading scholars in the field of computational mechanics.

Looking back on his experience as a doctoral student, Seleson enumerated the things he enjoyed about DSC and why he's glad he came to this program in Computational Science. "We have the facilities and tools needed for doing scientific computing. Some of the simulations we performed require a large amount of memory and computational time. Unless you have a computer cluster to do high performance computing, those simulations are not feasible. Lots of the fracture simulations I was running on the computer cluster were possible because DSC has such advanced computing equipment. I enjoyed having a Visualization Laboratory and being able to produce three-dimensional movies that showed visual results of my simulations. If new students wanted to come here, I would tell them that if they want to do computational applications of science, this is the right place to be."



Left, Below: Seleson presenting his research on July 20, 2010

SC Students Rock in Intramurals

Scientific Computing grad student Michelle Perry saw the need for some summer fun, and organized intramural sports teams for the department. Team Scientific Computing participated in several intramural competitions including soccer, kickball, wallyball, volleyball, dodge ball and flag football. Student participation was high, and the dodge ball team formed an alliance with Physics, and renamed the team Scientific Computing and Friends.

Right: Fierce competitors at volleyball
Below: After a soccer victory
Below Right: Ready for dodge ball

Intramural participants include Ariel Azoulay, Evan Bollig, Ben McLaughlin, Myrna Merced-Serrano, Michal Palczewski, Michelle Perry, Olmo Zavala Romero, Pablo Seleson and Arsia Takeh

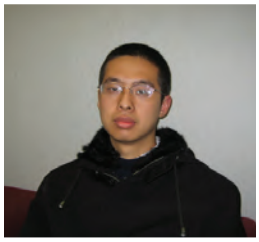
New Faces come to DSC

STUDENTS

For many years, Ariel Azoulay lived in Buenos Aires, Argentina, but moved to Boca Raton, Florida when he was sixteen. He finished his last two years of high school here, then obtained his bachelor's degree in

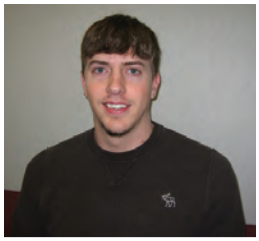
Pure Mathematics and Actuarial Science from FSU. He joined Scientific Computing to pursue his graduate studies and is working towards his master's degree. Ariel's areas of interest include computational mathematics, numerical linear algebra, optimization and optimal control. His current advisor is Janet Peterson. In his free time, he enjoys hanging out with friends and family, watching movies, playing sports, reading and writing.

Shengxu Xia hails from China where he received his B.S. and master's degrees in Mechanical Engineering from Hohai University in Nanjing. His master's thesis was entitled, Discrete Element Method for Simulating the Fracture Process.



Shengxu came to DSC in January to pursue the doctor of philosophy under the direction of Anter El-Azab. Currently, his research interest is dislocation dynamics, a topic that has many implications for properties of materials. Shengxu has many hobbies, including table tennis, flight simulation, and – if there's enough time – movie watching.

Although he was born in Bluefield, WV, Ryan Deskins and his family moved to Tennessee when he was very young. Ryan received his Bachelor of Science degree in Physics and Mathematics from East Tennessee State University in Spring 2008. Afterward, Ryan applied and was accepted to the graduate program in physics at FSU, and began his master's degree in the Fall of 2008. While in the physics department, he studied Monte Carlo simulations on a two-dimensional Ising model. Subsequently Ryan submitted a preprint of a paper titled 'Kinetic Monte Carlo Simulations of a Model for Heat-assisted Magnetization Reversal in Ultrathin Films' to the Journal of Magnetism and Magnetic Materials. Ryan came to Scientific Computing in Spring 2010 as a master's degree student, and works with Anter El-Azab as a research assistant. He plans to use Monte Carlo simulations to investigate the role of defects on lattice thermal conductivity. Ryan is a long-time video gamer, and uses video games as a form of relaxation. At the end of the day, he likes to play first-person shooters on his PlayStation3 and enjoy a good beer.



POST-DOCS

Liying Wang studied at the College of Water Resources and Hydroelectric Engineering at Wuhan University in China; she finished her doctorate in December 2007. In her research, she experimented with simulating the transformation and transport of nitrogen and phosphorus in saturated and unsaturated soils. Liying is working with Ming Ye as a post-doc, doing research in uncertainty analysis of groundwater modeling.
Liying loves traveling, reading and movies. She enjoys her work and has learned a lot since coming to DSC. Getting to know the people here has been particularly rewarding for her, as she enjoys meeting and interacting with everyone.

Shengyu Wang joined the department as a post-doctoral research associate in March 2010. Currently, she is working with Anter El-Azab modeling microstructure evolution in irradiated materials using phase field simulation methods. Shengyu completed her Ph.D. in 2010 from Carnegie Mellon University in Pittsburgh, PA. She gained experiential and computational skills during her doctoral studies in materials science and engineering at

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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.

CMU. Her dissertation research involved Monte Carlo simulation and modeling of subgrain structural evolution in aluminum alloys based on EBSD (electron backscattered diffraction) experimental observations. Before studying at CMU, she obtained her masters degree in Mechanical Engineering from Louisiana State University where she studied the grain growth phenomenon in nanocrystalline materials using molecular dynamics simulation methods. Shengyu came to the US from China in 2003 to do her master's and doctoral work.

Shengyu enjoys living in Tallahassee with her husband and daughter. She likes classical music, playing outdoors, and parties. She looks forward to making new friends and having more fun in the Sunshine State.

STAFF

Brent Woodruff grew up in the foothills of North Carolina, where he graduated from Surry Community College before transferring to Appalachian State University. While at ASU, he completed a bachelors degree in Applied Mathematics and Computer Science and a Masters in Mathematics. In 2005, Brent began working full time in Technology Support Services, ASU's technology office. His primary duties were redesigning the support website, and implementing the university's Content Management initiative and Support Ticketing System.

In his free time, Brent enjoys playing board and video games, especially titles for the Wii and retro DOS adventure games, and he is reading Will and Ariel Durant's eleven volume series "The Story of Civilization." Brent and his wife Celestine enjoy caring for a few transplants from a local garden on their deck, and are planning a small container vegetable garden of their own for next year.

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