Department of Scientific Computing

Spring 2009

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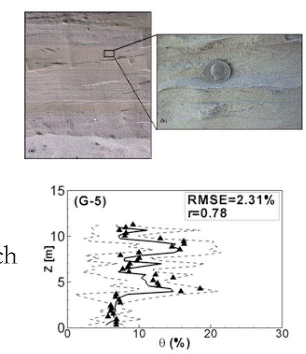
Computational Protection for Groundwater Resources

Undeniably, water is one of the most important resources on earth. Its countless uses and vital nature make it indispensable to plants, animals and humans – in fact, to all living creatures. With a resource so critical to survival, getting and keeping water clean and contaminant-free is a state and national priority. That's where Ming Ye, with funding from the United States Department of Energy, the Department of Defense, Oak Ridge National Laboratory, the Florida Department of Environmental Protection, and the FSU Institute for Energy Systems, Economics and Sustainability joins intellect, ingenuity, science, mathematics, and data in a concerted research effort.

Ye, an assistant professor at the Department of Scientific Computing, developed and whetted his interest in hydrology and water resources while a doctoral student at the University of Arizona, a place squarely in the arid Southwest, where water scarcity drives, among other things, public policy. Since leaving the desert southwest and coming to FSU, Ye has focused on research and funding that helps him continue finding ways to mitigate problems – often manmade – caused by water and water quality. Hydrological processes behind these problems are multiscale by nature, varying from individual molecular to ecosystem and from nanosecond to millennium. Modeling the hydrologic processes in the open and complex hydrologic system is challenging. It requires a solid understanding of the bio-hydro-geo-chemical processes and their interactions, as well as advanced mathematical/computational tools for quantitative predictions. On the other hand, relative to the problems being tackled, observations are always sparse and knowledge is often limited. Therefore, when model predictions are used for decision-making, assessment of predictive uncertainty is necessary. Uncertainty quantification is one of Ye's major research interests.



Figures illustrate research at the Hanford, WA site (DOE). Model shows how contaminants move in soils before reaching groundwater. Part of the difficulty of modeling at this site is the multi-scale soil heterogeneity as depicted in the top figure.

Presently, Ye is the PI (principal investigator) or Co-PI on more than a half-dozen grants specifically targeted to study and address water quality or the impact of water on the environment. The grant funds he receives help him study a variety of water quality issues: how coastal hydrologic systems change with potential sea level rise under future climate conditions and what those changes mean for the surrounding population; how contaminants react geo-

(See Groundwater, page 3)

Max Gunzburger, DSC Chair

From the Chair

Time has flown by. The Department of Scientific Computing is now one year old and has had a very good first year. We continue to be recognized by our peers as a leading unit for advancing research in computational science and engineering. Our graduate degree programs have gained international recognition and we are repeatedly contacted by other institutions for advice on how they can emulate what we are doing at FSU.

Our success during our first year builds a foundation for even greater things in the future. In particular, we are in the midst of finishing the design of an undergraduate degree program that we plan on offering beginning in the Fall 2010 semester. We are very excited about bringing undergraduates the same type of training that we have successfully given to graduate students. In anticipation of the undergraduate program, we have already developed several undergraduate courses; during the next academic year we are offering courses in game design, scientific computing, and symbolic and mathematical computations.

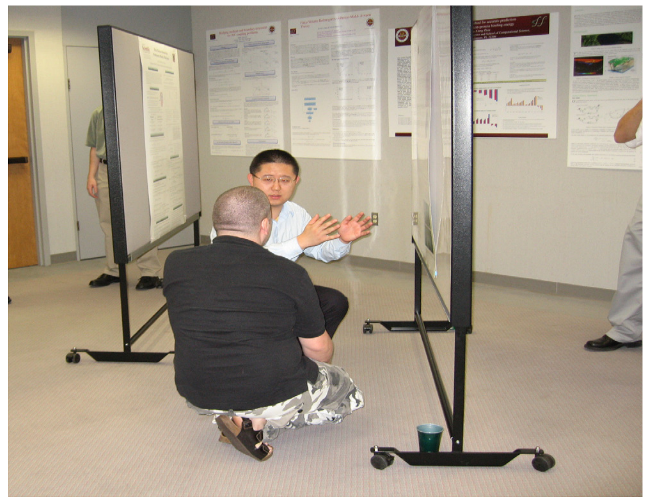
In this second newsletter as a department, we return to featuring the research of our faculty and their students and postdocs as well as some newsworthy events. We are particularly proud of the Xposition 2009 that recently took place and at which Department of Scientific Computing students presented posters describing their research. The diversity and quality of the research our students are engaged in is truly spectacular! Collectively, their posters provide conclusive hard evidence that our degree programs in computational science provide the type of training that is needed for students to make useful, practical, and innovative contributions to the solution of scientific and engineering problems.

Chair, Department of Scientific Computing

Research on Display at Xposition 2009

After late nights and early mornings running computer simulations, testing algorithms and gathering data, DSC graduate students took a break from research to put together posters, laptop presentations, and 3-D representations of their research for the 4th Graduate Student Research Xposition. Twenty-two masters and doctoral students showcased a portion of the research they've done over the last year on April 14, 2009. The Xposition was held in 499 Dirac Science Library.

This year, the students' research was particularly well-developed and diverse, demonstrating advances in basic theory and experimental research with topics relevant to computational science. Some projects introduced new methods of studying long-time problems. Other research took current thinking on a particular topic one step forward. And still other projects brought a fresh perspective to the field by posing completely new theories and hypotheses. The range of algorithmic invention and application problems represented by the posters is truly remarkable. Among the presentations were projects which focused on data storage, metal strength, stellar explosions or supernovae, overflow in oceans, classification and prediction markets, hydrologic modeling, and graphical user interface generation. The posters reflect the breadth as well as the depth and quality of the research carried out in the DSC, and speak to the high standards the students and their faculty advisors consistently display. For now, it's back to the lab until next Spring. For more information, including photos, posters and abstracts, log on to www.sc.fsu.edu.



Xi Chen and Geoff Womeldorff discuss Xi's peridynamic modeling research

Groundwater

(continued from page 1)

chemically and what stable conditions of the reactions are for contaminant remediation to be effective; or how high performance computing can be used for hydrologic modeling that is possible using a single processor. Results of these types of studies are indispensible to federal and state government agencies for water resource management and environmental protection. For example, his research supported by the Department of Defense will estimate potential losses to the drinking water supply caused by sea level rise, which increases the salinity of both surface water and groundwater through saltwater intrusion. His research funded by the Department of Energy will identify the dominating physical, chemical, and biological processes that control uranium transport to groundwater, a human radionuclide pathway. This process identification will help federal and state agencies optimize limited resources to study the most critical processes, monitor the most likely pathways threatening human health, and make sciences-based and scientifically defensible decisions.

Although each study is different, a frequent and critical component of Ye's research is the use of high intensity computation and parallel computing. "Some of the projects I have absolutely require high performance computing. In fact, I was specifically awarded at least one grant because of the HPC facility we have here at the university." (See related story, page 4.) Numerical simulations, modeling analyses, and computational algorithms are all computationally demanding, and the technological and computing facilities at FSU and DSC help make Ye's studies possible. "A problem run on the HPC could take a few hours, whereas if that same problem were run on a regular PC, it could take years."

James Wilgenbusch, HPC Director

Computing
HPC Visualiza-
tion Laboratory
Hosting SLAs
CLUSTERS Sup-
port Management
TECHNOLOGY High
Perfomance
Computing
DSC Technical Staff
Visualization Lab-
oratory

Above: Ribbon cutting on the HPC facility
Below Right: Staff enjoying state-of-the art 3D projection

Technology for a Research & Learning Community

Dennis Slice doesn't have far to travel when he delivers a lecture on morphometric analysis to anthropology students at the University of Vienna. He simply walks from his office on the first floor of Dirac Science Library to the fourth floor in the same building. There he enters room 499, puts on a microphone, and with the help of the technical support staff, uses the Department of Scientific Computing's (DSC) AccessGrid resources to appear simultaneously to students in Tallahassee and Vienna. AccessGrid is an opensource system for tele/video conferencing.

Slice's simulcast is just one illustration of the usefulness and technological possibilities available to the DSC faculty. Gordon Erlebacher uses the Visualization Laboratory for his research and to teach his students strategies to visualize scalar, vector and volumetric fields. Ming Ye uses the High Performance Computing facility to study the pollution and contaminants in groundwater. These are just a few examples of ways DSC faculty – and many other professors, staff and departments across the university – are using the DSC computing powerhouse for research, simulation, teaching, modeling and general operations.

According to Jim Wilgenbusch, Associate Director of the DSC and Director of the Shared High Performance Computing (HPC) facility, our computing facilities are scalable, comprehensive and versatile, and consist of four key components: the HPC, hosting services, technical support and the Visualization Lab. The first piece, the HPC, became a reality in 2007 and immediately became an indispensable computing resource for researchers who study problems requiring intense computation.

"A major focus of our technical efforts is in providing a robust and scalable HPC system to the entire university research community," said Wilgenbusch. "Intense computation is a fundamental requirement when performing research involving algorithms or complex data modeling. That's why we chose this particular set up." The HPC provides a computing platform for multidisciplinary research in a cost sharing environment. In the 18 short months the HPC has been operational, seven departments, including the Center for Ocean-Atmospheric Prediction Studies, Engineering, Scientific Computing, Institute of Molecular Biophysics, Biology, and Meteorology have purchased shares in the HPC, and over twenty articles are already in print with the help of the facility. "We're on our second upgrade cycle as of August (2008). During that upgrade we added four new groups probably because they saw what others were accomplishing with the resources and support that we are providing at HPC." HPC is already preparing for the 2009 upgrade at which time some new groups will join the HPC, including members of the Department of Physics along with researchers from the National High Magnetic Field Laboratory.

The second component of the DSC computational powerhouse combines server software and hardware with systems hosting and management. By offering other university units the opportunity to free themselves from the purchase and/or daily maintenance involved in having servers and data centers, DSC provides a welcome service to FSU. "The second service we offer to our faculty and other members of the university is that we host and manage clusters and database services in our data center on the fourth floor of Dirac Science Library. We work with departments to create a service agreement that provides them with a stable research platform and we leverage the tools and talents of our technical staff to effectively manage their system and to make available any unused cycles on the systems that we agree to support." Wilgenbusch and his staff work with departments that have varying hosting needs. Some smaller units have small computing needs and few staff, while others have and require higher level resources and management.

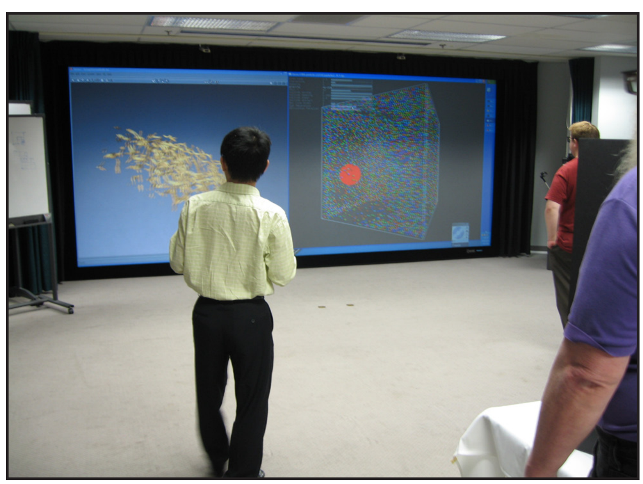
Following hosting and management, there's the third technological aspect. The third piece of DSC computing is, "…. the technical support which includes high level systems administration and instruction through technical workshops that are hosted in our computer classroom and seminar room. Some of the workshops we've done over the years have been very high level." Wilgenbusch and his staff frequently provide continuing education to the FSU community. The workshops range in depth and complexity – from "High Performance Computing 101" and "Supercomputing in Plain English" to more computationally and technically dense topics. Sponsoring these events positions DSC to extend its wealth of high-level knowledge more fully to the sciences and other interested university affiliates.

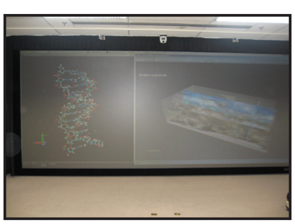
"Finally, there's the visualization component of what we provide. Two years ago Gordon Erlebacher, myself and three other PI's (principal investigators) were funded by the NSF through a major research initiative, to develop a new state-of-the art system and facilities for delivering 3D content to multidisciplinary researchers." The Visualization Lab provides faculty and research scientists with tools to help explain complex phenomena. Visualization permits faculty, students, and other research scholars to analyze data, extract information/features, correlate that information, and display their data in a meaningful way.

Not only are on-campus organizations utilizing the technology services offered by the DSC, but the scope of service provision has expanded beyond the boundaries of FSU's campus. DSC recently negotiated a contract with Port St. Lucie-based Torrey Pines Institute for Molecular Studies. The institute recognized the attractiveness of a university alliance, and began to make arrangements for contracting services through the HPC. This provides not only excellent computing facilities for Torrey Pines, but also includes the possibility of future research collaborations with FSU scholars.

DSC's comprehensive and powerful computing facilities are poised to meet the current and future computing needs of FSU and the larger research community. Wilgenbusch puts it this way, "We attempt to consider the full spectrum of what is required to support meaningful computational work, from the physical/environmental requirements for hosting hardware to the technical support requirements of how best to deliver and maintain specialized scientific software packages and libraries. The key is that we don't overlook the details so that everything is covered for a broad-base of application requirements."

For more information, log on to:
www.sc.fsu.edu/vislab
www.hpc.fsu.edu/





Graduate Students Awarded Summer Internships

Evan Bollig

Evan Bollig, a DSC doctoral student, has accepted a summer internship at the National Center for Atmospheric Research in Boulder, CO. His assignment is at the Computational and Information Systems Laboratory (CISL), where he will work under the direction of Jose Garcia and Rory Kelly on the project, Accelerated Computing Model Development. The objective of the project is to evaluate the use of accelerators for a 2D cloud-scale model embedded in the columns of a large scale 3D global atmosphere model. Evan will work on porting an existing cloud model to a GPU, and implementing an accelerated version of the model to run on NVIDA graphics hardware. This approach moves the heavy computation to high performance hardware, thereby reducing the computation costs. At DSC, Evan works under the direction of Gordon Erlebacher.

Doug Jacobsen

From May through August, Doug Jacobsen will live in Los Alamos, New Mexico where he will work with Todd Ringler and Mark Petersen at the Los Alamos National Laboratory. Doug and his colleagues will explore the effect of using various grid structures on resolving the physical process called overflow. Overflow occurs when dense, cold water overflows from a basin; it is responsible for the majority of the oceans' dense water and for the creation of many currents. Doug will use HyPOP to test a variety of grids to ascertain how each grid affects the outcome of the overflow data and which grid provides optimal results. The goal to is determine the optimal grid structure for resolving the overflow process in a large part of the North Atlantic, in particular, the Denmark Strait and Faroe Bank Sea Channel. Doug is a DSC master's student working under the direction of Max Gunzburger.

Steve Henke

For the second consecutive summer, Steve Henke is interning at the United States Army Research Laboratory in Aberdeen Proving Ground, Maryland. Steve is slated to work in the Computational and Information Sciences Directorate under the direction of Dr. Peter W. Chung. His project will focus on developing a computer model to investigate surface morphology of ferroelectric oxides with mobile charged point defects. An understanding of surface morphology in these materials is essential to the development of next generation electrical sensors and devices. Steve will be in Maryland most of summer, but will take some time to attend USNCCM, a computational mechanics conference in Columbus, OH and the ICMR Spring School on the Transport Properties of Oxides at the University of Florida in Gainesville. Steve is a master's student under the direction of Anter El-Azab.

Jennifer Murray

Geoff Womeldorff

Jennifer Murray has been selected to participate in the Summer Research Institute at the Pacific Northwest National Laboratory (PNNL) in Richland, WA. The internship begins May 18th and continues through August 7, 2009. Jennifer will work under the direction of Dr. Eric Bylaska, a senior research scientist in the WR Wiley Environmental Molecular Sciences Laboratory / Environmental Spectroscopy & Biogeochemistry Facility at PNNL. Her summer project will focus on the development of quasicontinuum methods for electronic structure calculations of nanocrystalline systems with Density Functional Theory (DFT), a quantum mechanical theory commonly used in physics and chemistry. This investigation is motivated by the need to extend the applicability of DFT methods to crystalline systems with numbers of atoms far beyond what can be treated computationally using current DFT techniques. The model reduction technique is based on direct minimization of the energy functional of the electronic system with respect to either the electron density in the case of Orbital-Free DFT method, or with respect to the one-electron wave functions in case of Kohn-Sham DFT approach. Jennifer is pursuing a master's degree, and works under the direction of Anter El-Azab.

Geoff Womeldorff will spend his summer working on Roadrunner, the world's first petaflop system, and currently listed by the Top500 list (www.Top500.org) as the fastest supercomputer in the world. In June, Geoff is headed to Los Alamos National Laboratory (LANL) in Los Alamos, NM for a summer internship. He will work with Todd Ringler, a member of LANL's Climate, Ocean and Sea Ice Modeling Group, and will spend his time writing code related to POP and HyPOP, two ocean circulation models. This work will extend the research on ocean models and help develop new numerical methods for use in climate system modeling. Specifically, Geoff will spend the summer developing algorithms for the Cerrillos hybrid architecture. The internship at LANL will continue from June 1 until the end of August. During this three month period, Geoff will be exposed to the cutting edge of computing in Roadrunner, other highly advanced computational facilities, knowledgeable, leading scientists, and the full smorgasbord of resources available at one of the largest science and research institutions in the world. "Being in an environment where I will be exposed to the cutting edge of computing is exciting, and sure to be valuable no matter which path I pursue after graduation."

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

Gunzburger Selected Charter SIAM Fellow

The Society for Industrial and Applied Mathematics (SIAM), the leading applied mathematics society in the world, has named Max Gunzburger, Francis Eppes Professor and Chair of the Department of Scientific Computing, as one of its charter group of fellows. This award follows a series of prestigious recognitions for Gunzburger. In 2008, he was awarded the W.T. and Idelia Reid Prize in Mathematics. In 2007, the International Journal of Numerical Analysis & Modeling dedicated a special issue to Gunzburger in recognition of his many contributions to the field of mathematics. He served as editor-in-chief of the SIAM Journal on Numerical Analysis, the leading journal in computational mathematics from 2000 through 2007.

The SIAM Fellows Program was recently approved by its membership as a means of accomplishing several valuable goals: to honor SIAM members who are recognized by their peers as distinguished for their contributions to the discipline, to help make outstanding SIAM members more competitive for awards and honors when they are being compared with colleagues from other disciplines, and to support the advancement of SIAM members to leadership positions in their own institutions and in the broader society. As SIAM is becoming the first mathematics society to institute a fellows program, the selection criteria for this honor was limited to a small, but accomplished population of mathematicians, scholars and scientists who had been previously singled out for notable accomplishments in the field. Gunzburger was selected for his well-known and often cited research contributions to computational and applied mathematics and for his many years of distinguished service.

Until now, mathematics societies worldwide, including, in the US, the American Mathematical Society, the Mathematical Association of America, and SIAM, have shied away from naming fellows of their society. Gunzburger stated, "There has been a growing awareness among mathematicians that honoring the most accomplished among their peers by naming fellows, as professional societies do in many other disciplines, is worthwhile."

The charter group of fellows will be recognized at a luncheon held on July 7 during the SIAM Annual Meeting in Denver. Gunzburger added, "To be among the first group of applied mathematicians selected by SIAM to be a fellow of the society is a great honor. It is quite humbling to be listed among the other charter fellows and to have this honor bestowed a year after receiving the Reid Prize." He went on to say, "As is the case for almost everyone receiving such recognition for their professional accomplishments, whatever I did to deserve being named a SIAM fellow was greatly aided by many students, postdocs, and colleagues, all of whom I warmly thank."