Department of Scientific Computing

Fall 2011

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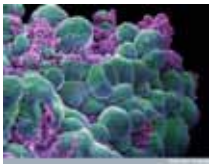

Combining Computer-Aided Diagnosis and Systems Biology to Detect and Treat Cancer

Breast cancer is one of the most common and deadly cancers among women, with over 200,000 new cases in 2010 alone. Statistically, breast cancer affects one in eight women during their lifetimes. Because of the high incidence of the disease, physicians hope to discover the cancer while it is very small, as providing treatment during the earliest stages increases the likelihood of successful arrest and removal. Traditionally, dynamic magnetic resonance imaging (MRI) of the breast, reported to be a highly sensitive diagnostic method for cancer detection, has been used for this purpose. MRI uses magnetic and radio frequencies to visualize structures inside the body, and gives physicians higher quality images when compared to x-rays and some other diagnostic tools.

DSC Professor Anke Meyer-Baese however, is using newer, more refined methods in her research to study alternative ways to improve the images doctors use to evaluate breast health. Specifically, Professor Meyer-Baese's research assists in the important work of early detection by providing further evaluation of clinically, mammographically and sonographically occult cancers that are timely, comprehensive and accurate.

Driving Meyer-Baese's research are two approaches that capitalize on the success of computer-aided design in conventional x-ray mammography. The first, single-breast imaging protocols with high spatial resolution, offers a meticulous analysis of the lesion's structure and internal architecture. This diagnostic tool can distinguish between benign and malignant lesions, a task that previously was a separate and time-consuming step in the diagnosis. The second approach, lesion differential diagnosis in dynamic protocols, is based on the assumption that benign and malignant lesions exhibit different enhancement kinetics (energy). These diagnostic techniques motivated the research of automated diagnosis techniques in breast MRI to expedite diagnostic and screening activities. "These methods provide better information and faster diagnosis than the previous tests. This allows doctors and patients to make decisions on treatment almost immediately," said Meyer-Baese.

An additional element of Meyer-Baese's research is her exclusive focus on very small tumors. "We design and evaluate a computerized analysis for diagnosing small breast masses. Our primary focus is on tumors with a diameter of only a few millimeters." Studying very small tumors can be very beneficial for the patient, as early detection and action

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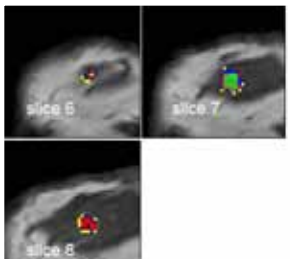

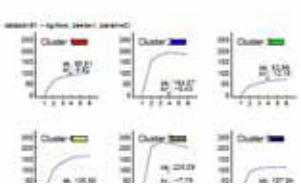

Figures above: Segmentation method based on the "neural-gas" network applied to data set #1 (malignant lesion, DCIS) and resulting in six clusters. The left image shows the cluster distribution for each slice ranging from 6 to 8. The right image visualizes the representative time-signal intensity time curves for each cluster.

Scientific Computing in Psychology: Spring 2012

Beginning in the Spring, Scientific Computing will embark on a new venture, partnering with the Department of Psychology to offer a 4000-level course entitled *Computer Applications in Psychology with Laboratory*. The course is recommended for all psychology majors who have or will have completed two prerequisites, Research Methods in Psychology (PSY 3213C) and the computer literacy requirement, prior to the semester of enrollment. The course was developed by Scientific Computing faculty specifically for psychology majors, with input from the psychology faculty. The course will provide each student with practical knowledge of R, a power, open source programming language used for its statistical and graphics capability.

In the course, students will apply programming, computational and research elements to subjects important to the field of psychology. Each week will be dedicated to one topic related to programming, such as complex searches, image and audio manipulation, or data analysis, each selected to provide psychology students with practical skills and tools that can help them in their research, and make them more competitive for graduate/professional school and/or jobs. Professor Gordon Erlebacher, Professor and Interim Chair, will teach the upper level course.

Students will use psychology data sets in the class which will allow them to formulate and structure individual exercises using familiar and relevant concepts. Course curriculum will include concepts of the language R, data protection and backup, reading and writing datasets, preparing data for analysis (and conducting simple statistical tests), data restructuring, Excel queries, internet searches, signal and image manipulation, visualization of experimental data, image databases and handling audio data.

The 4-credit hour class includes a lab, where students will apply the material presented in lectures and complete weekly assignments. The course has three different laboratory sections, giving the students wide flexibility in scheduling. Students will be graded exclusively from their weekly lab report submissions, each structured as a research paper.

Scientific Computing graduate students Ben McLaughlin, Andrew Young and Nathan Lay will serve as Teaching Assistants for the course. For more information about the class go to http://www.psy.fsu.edu/undergrad.prog/Computer_Apps_Psych_Syllabus.pdf. For information about Scientific Computing undergraduate courses, go to http://www.sc.fsu.edu/undergraduate/courses.

Top to Bottom: Graduate Teaching Assistants Andrew Young, Ben McLaughlin and Nathan Lay.

New Social Network Established

FSU's shared-HPC web site just got a little more social. The new social net work site, HPC Community, resembles social networking sites like Facebook and LinkedIn, only this site is all about helping students, scholars and scientists do research on HPC resources. Tools like this are increasingly becoming popular to help accelerate the quality, engagement, scope and completion of scientific research. HPC Community facilitates sharing with peers to answer questions, gather advice on algorithms and materials, pool knowledge and ideas, and increase the number of scientific minds thinking about specific research problems. A primary advantage of HPC Community is the creation of a virtual scientific commons accessible to any researcher in any field of science.

HPC Director James Wilgenbusch and his staff have already begun to create structure and organization around the new site. "We've already started several groups under HPC Community to help focus the discussion and welcome other members to start groups of their own."

Like other social networking sites, HPC Community is universally accessible and easy to use. Getting connected is as easy as clicking the "HPC Community" link under the left hand menu of the HPC web site - www. hpc.fsu.edu.

Whether they're working on Next-Gen sequencing or High Energy Physics, HPC Community is a great way for HPC users and research affiliates to collaborate, share successes, ask questions, and move research forward.

Image Below: InfiniBand processor nodes

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increase the rate of cure, but the small size presents a special challenge, as the lesions contain only a small number of voxels, and morphologic criteria is hard to evaluate. Additionally, the value of dynamic MRI and of automatic identification and classification of characteristic kinetic curves is not well established in small lesions when clinical findings, mammography, and ultrasound are unclear.

To overcome these problems, Meyer-Baese, her graduate students, and other collaborators employ a "neural-gas" network as a quantization method that focuses strictly on the observed complete MRI signal time series. This solitary focus enables a self organized, data driven segmentation of dynamic contrast enhanced breast MRI time series with respect to fine grained differences of signal amplitude and dynamics, such as focal enhancement in patients with indeterminate breast lesions. This method is developed, tested, and evaluated for functional and structural segmentation, visualization, and classification of dynamic contrast-enhanced breast MRI data. "These studies are highly complex and require the assistance of professionals from the medical and academic fields," said Meyer-Baese. "We believe the results, though, are very important for cancer research."

Multi-modality diagnosis techniques are more and more replacing traditional medical imaging for breast cancer detection. Newly emerging advances in both intelligent cancer detection systems and lipidomics technologies offer an excellent opportunity to detect tumors and to understand regulation at the molecular level in many diseases such as cancer.

Because brain tumor (glioblastoma) is a secondary tumor form of breast cancer, Meyer-Bases includes its study in her research. Glioblastoma differs from other tumors and is characterized by uncontrolled motile cells that can migrate as well as proliferate. Thus, despite recent advances in chemotherapy, radiation therapy and surgical resection, these malignant primary brain tumors, are almost always fatal. More promising therapies are expected through gene therapy.

Mathematical modeling in lipidomics will play an important role in the study of biochemical mechanisms, especially in cancer therapeutics. Furthermore, the crucial task remains to integrate heterogeneous datasets from lipidomic, transcriptomic and proteomic data and to build powerful models that describe the lipidomic process and its regulation. Dr. Meyer-Baese developed and tested novel graph-clustering techniques applied to the interpretation of lipidomic data sets in response to several therapeutic combinations. Thus, the lipidomic correlations can be interpreted as a characteristic fingerprint of the underlying system.

Scientific Computing Grads Begin a New Chapter

Within weeks of completing her degree in May, SC graduate Jennifer Murray had a position at Infinity Software, a local leader in custom software development for government and the private sector. Jennifer is a Business Process Analyst, a broad term, she says, for writer/editor, content developer, and information organizer, a job in which she constantly uses math, science, research and analysis skills honed at Scientific Computing.

"Infinity has a pretty wide range of projects and clients. They develop and maintain business software and websites, assist clients with development of new business practices, organization, and do website and logo design. I've been working on a team that develops educational materials for K-12 online resources, like the FCAT Explorer and the Florida Virtual Schools programs. I write and revise lesson and assessment content in subjects like science, math, and civics."

Jennifer's current project has two goals. The first is to assist teachers in the classroom, providing Florida students with a way to earn credit in classes that may not be traditionally accessible to them. The project also helps prepare students to pass state required teaching exams. Jennifer's experience as a teaching assistant in Web Design and Java classes has helped her to navigate the learning curve quickly. "I think my computational science experience has given me an overall picture of what is involved in software development and how the area of computer science breaks down into different domains. This high level view has helped me understand the work that is done at my company," she said. "I also think that my M.S. degrees are what helped me get this job in the first place."

Jennifer's research at Scientific Computing under the direction of Anter El-Azab directly ties into her new position. Her research project focused on developing the mathematics, algorithms, and a basic test program to test an idea for reducing the complexity of an optimization problem. This problem required the minimization of the electronic structure energy of a nearly crystalline cluster of atoms. The goal was to find a more efficient way to calculate the ground state electron distribution in the cluster. It relied on the fact that atoms and their associated electron densities are usually packed into a periodic, or repetitive, arrangement in solids. In real solids, especially small solids with large surfaces, like nanoparticles, or solids with defects, this periodic arrangement strays from a true, strict, periodic arrangement.

"Prof. El-Azab's idea was to use an interpolation method, like finite element interpolation, to approximate the way the electron density would vary across a group of atoms. The key to this idea was that although the electron density can have a complicated physical distribution around each nucleus, when you "measure" the electron density in an atom in this nearly periodic arrangement and then "measure" it at the same spot but in neighboring atoms, the measured values are nearly the same," Jennifer explained. They vary only slightly, depending on the degree of deformation of the periodic structure, and it was proposed that this variation can be captured by an interpolation function, like a linear finite element interpolation function.

Using this idea in conjunction with previous work by collaborators, Jennifer and Professor El-Azab developed an interpolation scheme that used two levels of interpolation, the first at a coarse scale across groups of atoms, the second at a fine, subatomic scale. Jennifer developed the math formulas and algorithms to compute the electron energies based on Orbital-Free Density Functional Theory. She also wrote a program that computes these energies based on the algorithms

she developed.

In remembering her time in the program at Scientific Computing, she considers her most important experiences were the interactions she had with people from various backgrounds.

"I really gained an appreciation for other fields in science, in business, and in life in general from the conversations I had with classmates and professors from various fields in DSC. The computational science program opened my eyes to new ways of looking at the world. I think that new perspective, in addition to the rigorous mathematics and numerical methods, is what I carry away with me and what helps me in the development of my own professional goals."

Doug Jacobsen started as a master's student in the Fall of 2007 without knowing specifically what he wanted to do for research – he just knew how much he enjoyed using computers for scientific topics. After his first year of classes, he started working with Max Gunzburger on a climate modeling project. In the climate modeling project, the research involved exploring the effect different choices of vertical coordinates and vertical mixing strategies have on a physical process known as Overflow. While doing this research, Doug became involved with scientists at Los Alamos National Laboratory and spent a summer internship there working on the project.

After finishing his Masters degree in Fall 2009, Doug shifted focus to the requirements for the doctorate. His work included a variety of topics from multi-resolution methods for simulation ocean flows, to parallel grid generation on the surface of the sphere. He studied Adaptive Mesh Refinement techniques using Spherical Centroidal Voronoi Tessellations. Adaptive mesh refinement techniques allow simulations to use a lower number of degrees of freedom while maintaining a higher accuracy. Doing so reduces overall computational costs in simulations.

Doug defended his dissertation in Summer 2011, and with all the requirements for the doctorate behind him, he recently began a postdoctoral position at Los Alamos National Laboratory. Doug will work with Phil Jones on co-design of numerical algorithms, which involves migrating existing algorithms to heterogeneous architectures.

"I thoroughly enjoyed my time at the Department of Scientific Computing. There are many gifted faculty members and students involved. I have been able to see three years of new students enter the department, and see the department change around all of us that have been involved. All in all, it has been a terrific experience, and I thank everyone who helped make it that."

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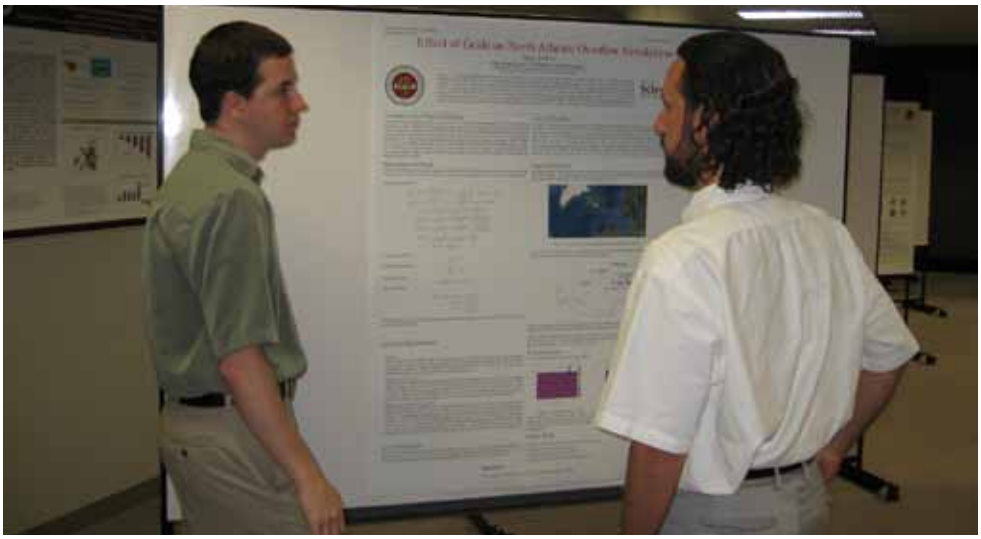

Doug Jacobsen and Pablo Seleson discuss Scientific Computing research at the grad student research Xpo.

New Undergraduate Lounge Accommodates Students

Scientific Computing's Undergraduate Lounge is now open! Located in Room 486, the Lounge was created for the department's undergraduate students as a place to informally gather, study, collaborate and relax. Room 486 was allocated as space for the Lounge late in the Summer, and recently has been reconfigured to accommodate fresh furnishings to include two desks, each with a networked computer workstation; a variety of seating and work areas, including a couch, a work table with chairs, and individual chairs; and a white board. The idea was to give students a multipurpose place they could call their own to wait between classes, informally discuss course projects, conjure insights, and connect with department faculty, post docs, grad students, and staff.

The students nicknamed the Lounge the War Room, and have made themselves at home by putting posters and course notes on the walls. The Lounge will be open and available 24 hours a day.

SC Welcomes New Staff

Maribel Amwake began as the department's new Academic Support Assistant in the Summer, strategically positioning her entry to learn the basics of the job during the calmest period of the academic year. Maribel came to Scientific Computing from the Arts and Sciences Dean's Office, where she worked as a receptionist for the Office of Student Affairs. While working as a receptionist, she learned College and University policies, provided computing trouble-shooting services for staff, created new forms, and gave direction and counsel to students.

Maribel is an FSU Theatre graduate, receiving her Bachelor of Arts degree in 2004. Shortly after graduation, she accepted employment at a local bank while simultaneously offering videography, videotaping and video editing services. Maribel left the bank and worked full-time as a business owner and videographer, but accepted a position with WFSU-The Florida Channel when the opportunity arose. Maribel left WFSU for the Dean's Office position.

As Academic Support Assistant for Scientific Computing, Maribel is responsible for a variety of duties related to both graduate and undergraduate students. For graduate students, she handles admissions-related processes, assists with course review and registration, manages the graduate student tracking system, and schedules oral preliminary examinations.

Current and perspective undergraduate students rely on her for counseling and advice regarding course selection and course schedules. Maribel also maintains all the student files and attends to other duties related to the day-to-day operations of the undergraduate and graduate programs. Earlier this Fall, Maribel was involved in student recruitment, attending FSU Day at Tallahassee Community College. "It was fun to talk to the students about our Department and our program at TCC. There were a few students who were very interested in our program and may even join our department in a few years when they come to FSU. Our display not only captured the students' interest, but the attention of many advisors from different FSU departments

Maribel has been married for almost 6 years to David Amwake, and has a thirteen-year-old Collie, Misty, and a six-year-old Cocker Spaniel, Dante. She enjoys reading, hiking, badminton, video games, movies, and video editing.

Donald Shrum came to Scientific Computing earlier this year, with an extensive computing background. Don earned both his undergraduate and graduate degrees at Florida State, being awarded the Bachelor of Arts in Creative Writing with a minor in Computer Science in 1998 and a Master of Science in Information Studies in 2004.

After completing his undergrad, Donny briefly worked for IBM in Tampa, then returned to Tallahassee for a position at the Florida Department of Education as a Systems Project Administrator. While at DOE, Donny was the technical lead for web-based database applications. In 2004, he completed the MS degree and returned to Florida State, accepting a position as an Application Developer and Designer at the Office of Technology Integration. There he performed tasks related to the Identify Management Group, the university's method of identifying and authenticating user IDs for 300,000 faculty, staff, alumni, students and student applicants. Before arriving at Scientific Computing, he was worked at the FSU Foundation as Database Administrator and Lead Programmer.

As Systems Programmer/Distributed Storage Specialist for the department, Donny supports the systems, programming and distributed storage requirements of the HPC, which helps develop a cyber infrastructure to support collaborative research activities among FSU, UF and USD.

In addition to his background in computing, Donny is an entrepreneur, licensed pilot and flight instructor.

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The department's mission is to be the focal point of science and computation at Florida State University. Gordon Erlebacher is the Interim Chair of the Department of Scientific Computing. He can be reached at 850.644.0143. 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.

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Since graduating with a Master's degree in Computational Science in May, Verónica Vergara Larrea has been working at Purdue University's Rosen Center for Advanced Computing as a Scientific Applications Analyst. Veronica's job is to provide consulting services to researchers across campus as well as support for users of their computational resources.

The Rosen Center is the research arm of Information Technology at Purdue. It provides advanced computational resources and services to support Purdue faculty and staff researchers. Rosen also conducts its own research and development to enhance the capabilities of these resources.

While at Scientific Computing, Veronica's research focused on parallel programming and grid generation. Her research was supervised by Max Gunzburger, and was centered on the development of a parallel algorithm for the construction of Delaunay Triangulations on the sphere. This particular kind of triangulation is of high interest to the scientific community because it can be used as an intermediate step in the generation of Voronoi Tesselations, an unstructured grid used in various numerical methods. The goal of the project was to be able to speed up the construction of Delaunay Triangulations in order to generate finer grids in less time. The algorithm was based on a serial Fortran package called STRIPACK and was written in C++ using MPI.

"Working with Max was a great experience," Veronica said. "He gave me the opportunity to pursue my interests and explore and test my ideas in the development of this project, and I am very thankful for that. One of the characteristics I enjoyed the most about the Computational Science program, was that I had the chance to work in a variety of fields, which I believe has given me a solid and broader foundation to work in this field. I think what had the most impact on my career, academic and professional, was working with Paul van der Mark at the High Performance Computing center during my TSG assistantship. Before that, I had never had the chance to work on a supercomputer, and even less thought about a career in the field. I really enjoyed working with everyone at DSC and HPC, and my experience wouldn't have been the same without them."