# Department

# Scientific Computing

### CONTENTS

of



Chair's Message



Beerli's Genetic Research



New Graduate Students



### Wang's Contribution Improves Image Segmentation Algorithms

Computers can perform certain data manipulation tasks more quickly and efficiently than any human ever possibly could. Some tasks, though, are exactly the reverse - easy for humans, but arduous and highly complex for computers to accomplish. One task where humans have an advantage is in identifying and understanding objects, then discerning meaning within a specific context. Although it requires complicated and interrelated processes, this type of recognition is one in which humans are superior.

Computer vision and image segmentation research are attempts to instruct computers to recognize, then accurately label objects and images. Doing so has multiple layers of complexity, because the computer has to recognize an image in context, discern between relevant and non-relevant information, then complete a task or tasks based on the interpretation of that useful information.

Using a computer to 'see' an object and distinguish it from its environment, however, is one stream of Scientific Computing Assistant Professor Xiaoqiang Wang's research. He studies Centroidal Voronoi Tessellations and their application to image processing, scientific visualization, computer vision and data mining. Centroidal Voronoi Tessellations (CVTs) are special Voronoi Tessellations that are generated from the geometric center of associated Voronoi regions, with respect to a specific density function.

Because these tessellations closely approximate patterns seen in nature, they are particularly useful in identifying images and variations in images by using computational algorithms. Practical applications of Wang's image segmentation research could be identifying or verifying a person through face recognition, comparing the structure of normal human cells to those that are suspicious or unusual, or locating objects [roads, waterways, mountains, canyons] in satellite images.

Spring 2012

"Segmentation is the basic problem in imaging and computer vision. It has been broadly used in many, many applications -- medical imaging, radar imaging, image reorganization, mine detection, and the like. It has also been applied in designing search engines for images, as it is very versatile, and highly utilitarian." Wang said.

EWCVT, continued on page 2



Images above are applications of the EWCVT to two images. The images are divided into three parts and show different superpixel densities.

# From the Chair

The Department of Scientific Computing is now four years old and growing. 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.

We have continued to build upon our success in the past two years by establishing a minor in Computational Science, along with a new course offered to the students in the Department of Psychology to help improve their skill sets in a difficult marketplace. Our flagship undergraduate courses, Game Design, and Introduction to Scientific Computing continue to garner interest across a range of departments at FSU. Without a doubt, the job prospects of our students improves markedly with a course program that emphasizes a mix of computing and practical applications, which defines computational science.

We have just concluded Xposition 2012, the best to date with over 25 presentations of student research, which shows a great range of diversity and uniformly high quality. Collectively, their posters provide conclusive 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 solve scientific and engineering problems.

In this Spring issue of the newsletter, we feature the research of some of our faculty, their students and postdocs. We also present those students who joined us in Fall 2011. They are excited and ready to participate in our program!

Gordon Erlebacher Interim Chair Department of Scientific Computing

#### EWCVT, continued from page 1

Wang, along with Jie Wang, now of Arizona State University and University of South Carolina Associate Professor Lili Ju, has contributed two important extensions to the field of CVT research. Although the classic centroidal model works well with uniformly colored images and objects, it is less successful in analyzing images with distinct color distribution or strong inhomogeneous intensity. Wang's research provides additional methods of analyzing images that incorporate image intensity information with the length of cluster boundaries.

"Some images, especially medical and satellite images, have inhomogeneous backgrounds and high variation in the foreground of objects. Traditional image segmentation methods easily confuse background and foreground objects."

The model Wang and his colleagues developed is called Edge-Weighted CVTs, an improvement that integrates image boundary information into the CVT clustering energy. The EWCVT model eliminates extraneous noise (unwanted data and information not relevant to the image analysis), is easy to understand and implement, and is better than the classic CVT model at segmenting images. Wang's model can be easily applied to multicluster image segmentation, an application that is unavailable in the classic CVT model.

"Before EWCVT was introduced, people used something called the Active Contours Method. This is an image segmentation method based on the Level Set Method required to solve partial differential equations. EWCVT can be used to get similar results with very low computational costs and more importantly, it is very easy to implement, because it does not need to solve a PDE."

continued on page 8

# Zhang Awarded Householder Fellowship



Guannan Zhang in the NY/Niagra Falls/Ontario area.

Graduation gifts came early for Scientific Computing doctoral student Guannan Zhang in the form of a prestigious post doctoral fellowship at Oak Ridge National Laboratory. Zhang is the recipient of the Alton S. Householder Fellowship in Scientific Computing, a national award to promote innovative research in scientific computing on advanced computer architectures and to facilitate technology transfer from the laboratory research environment to industry and academia through advanced training of new computational scientists.

Zhang will complete his doctorate in Computational Science next semester, but began the rigorous application process for the fellowship last year. "Since I had been planning to graduate in the Summer 2012 term, I applied for the Householder Fellowship at ORNL in December, 2011," Zhang said. "In February of this year, after I submitted my application and it was reviewed, I was invited on site to the lab for an interview which consisted of two parts. First, I presented my research to a group of scientists, then afterward, I talked individually with every

member of the Householder Fellow Search Committee." About two weeks after the interview, Zhang was informed he was selected as the 2012 Householder Fellow.

The award confirms Zhang's varied and extensive research portfolio which has focused on uncertainty quantification, numerical methods for stochastic partial differential equations, Bayesian analysis and its applications in geophysics and environmental science, high performance computing, and mathematical analysis of nonlocal models. Under the supervision of Professor Max Gunzburger, he has collaborated with a host of local and national scholars, and has submitted and published work in journals such as the SIAM Journal on Numerical Analysis and the Journal of Computational Mathematics.

In addition to his research, Zhang has been an active and key contributor to the field through his intellectual participation, contributions and presentations at meetings. This year alone, Zhang will present his research at a host of key conferences and meetings, including SIAM SEAS 2012, the SIAM Conference on Uncertainty Quantification, the SAMSI workshop on Uncertainty Quantification for High-Performance Computing, the SAMSI workshop on Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications, and the 2012 SIAM Annual Meeting. In years past, he has presented posters, offered workshops, and prepared various presentations.

The Householder Fellowship honors Dr. Alston S. Householder, founding Director of the Computer Science and Mathematics Division) at the Oak Ridge National Laboratory, and recognizes his seminal research contributions to the fields of numerical analysis and scientific computing. The fellowship promotes innovative research in scientific computing and to facilitate technology transfer from the laboratory environment to industry and academia.

# Beerli Studies Genetics with MIGRATE



Michal Palczewski, Haleh Ashki and Peter Beerli, April 2012.

Associate Professor Peter Beerli has a particular affinity for research. It appeals to his natural curiosity, and is independent and self-driven, with myriad possibilities. Beerli's research and teaching program is centered around patterns in genetic data which allow inference of evolutionary histories of populations. This research can be applied to understand genetic interactions among different human tribes, infection histories of influenza viruses or the fate of an endangered species. In one study, Beerli and his coauthors evaluated the origin of Mexican cave fish populations using microsatellite data. After statistically comparing cave settling characteristics, their research showed that cave populations are derived from two different surface stocks. Each of these two stocks colonized caves independently on at least two different occasions. Given these independent events, the similar phenotypes of the cave fish suggests repeated convergences.

Genetic data is often easily available, but the studies tend to be complex - - composed of many intricate, interconnected parts, utilize large, complicated data sets and require complex analyses. As an aid for his research and the research of others, Beerli has designed and created his own software, called MIGRATE.

"My computer program MIGRATE is one of the few computer programs for these types of genetic data analyses. Very recently we developed tools to compare different population genetic models that not only allow us to order a set of population models, but permits us to find appropriate models and exclude large numbers of improbable models that do not reflect the data very well. This process yields models with increased logical rigor and precision, saves researchers time and resources, and increases the validity of results," Beerli said.

Beerli will continue and extend his research on genetically structured populations with a recently received \$327,000 National Science Foundation grant. The proposed work builds on previous research that focused on developing tools to infer parameters of structured coalescence models and compare these models using Bayes factors, a Bayesian equivalent to likelihood ratio tests.

To use the full potential of this model comparison approach, they also will extend the available models in MIGRATE that currently accommodate a complex set of population substructures and estimation of parameters such as population size and immigration rates. These extensions will add estimators of divergence time of populations, and will allow inclusion of various recombination rates among DNA fragments along the genome. Once completed, the model framework will be very rich and will allow inference of complex biogeographic models that may help researchers understand the changes in distribution caused by climate change and human-induced landscape changes.

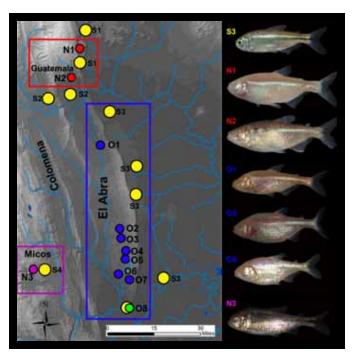
The model comparison framework may contain potentially complex models with many parameters that

are difficult to infer with accuracy. Beerli's group is working to improve algorithms that can be parallelized to run on fast graphical processing units when calculating probabilities for particular events, such as migration events or divergence events. Beerli's group has considerable experience in using his methods on cluster computers, such as the FSU highperformance-computing cluster; the distributed program can easily run on several hundred computers and calculate parameters using many independent genetic markers in parallel. All improvements will be built into the MIGRATE, so other researchers can

benefit.

**Currently MIGRATE has** approximately 2,500 registered users and more than 900 cited articles that describe Beerli's methods and programs. A large user-base results in many questions on how to run the software, how to analyze particular problems, how to read the output, and how to evaluate whether the assumptions for the methods and program are not violated. Beerli spends considerable time answering questions from the research community via the MIGRATE support group on Google. He also gives workshops around the world at institutions such as the Marine Biology Institute in Woods Hole, MA, the Smithsonian Conservation Genetics unit in Washington, DC, and the Molecular Evolution Workshop in Český Krumlov in the Czech Republic. In addition to his regular classes, he teaches several Python short courses at no charge over the Summer here at FSU.

For more information about Dr. Beerli, go to http://people.sc.fsu. edu/~pbeerli For more about MIGRATE, including the latest software updates and tutorials, visit http://popgen.sc.fsu.edu



The figure at left is a Map of the Sierra de El Abra region showing all the cave and surface collection sites. The colored boxes delineate major geographical regions as follows: El Abra region: O1 - O8 (blue & green circles); Guatemala region: N1 - N2 (red circles); Micos region: N3 (purple circles); Surface localities: S1 - S4 (yellow circles). Light blue lines represent different river systems in the area.

This image provides a visual representation of research by Beerli and his co-authors found in Bradic, M. et al., 2012. Gene flow and population structure in the Mexican blind cavefish complex (Astyanax mexicanus). BMC Evolutionary Biology, 12(1), p.9.

# New Students Come to SC

Before coming to Scientific Computing, doctoral student Qingguang Guan studied at Ji Lin University in Changchun China. He earned a Bachelor of Computa-



tional Mathematics in July 2009, and a Master of Numerical Analysis in July 2011. While at Ji Lin University, Qingguang taught Numerical Analysis of Stochastic **Differential Equations** and tutored high school students in mathematics. He has published papers in the science edition of the Journal of Ji Lin University, and in the IMA Journal of Numerical Analysis. Qingguang is advised by Max Gunzburger.

A Tallahassee native, SC Master's student John Jay Hogan attended New York University on a merit scholarship, earning a Bachelor of Arts degree in Urban Design in December 2005, then returning home to earn a Masters in Urban and Regional Planning in December 2007 from FSU. Afterward graduating from FSU, Jay worked professionally in urban design and urban planning.



Jay is pursuing the Professional Master of Science degree, and is in interested in two research areas - the application of genomic data towards the reconstruction of phylogenies and population dynamics and the use of bioinformatics in clinical practice. Currently, he is working with Alan Lemmon on phylogenetics research.

Jay enjoys teaching, and has tutored students in mathematics, algebra, calculus, statistics, biology, English, history, Public Administration and SAT/GRE test prep. When he has free time, Jay likes to spend it outdoors, playing guitar or piano, travelling or reading, and learning new skills.

### Benjamin J. Pomidor

is a Tallahassee native and recent FSU alum, graduating in May 2011 with dual BS degrees in Physical Science and **Biomathematics**. After experimenting with several different science areas, Ben enrolled in some programming courses offered by Scientific Computing. He enjoyed the course work and the environment so much, Ben decided to apply to the program. Currently Ben is working with Dennis Slice on research that applies an iterative closest point algorithm implementation in the



field of Morphometrics.

Although much of his time is spent writing programming code for classes and research, Ben has many other interests. He enjoys programming outside the academic setting, and is collaborating with his younger brother on an independent video game project. Ben enjoys playing video games, rollerblading, cooking and playing with his dog

Ph.D. student Kenneth James Soda, Jr. is originally from Monument, Colorado and attended high school in nearby Colorado Springs, Colorado. In 2009, he received his Bachelor of Science in Biology from Western



Washington University in Bellingham, Washington. Upon leaving Western, he briefly assisted the Invertebrate Zoology Department of the National Museum of Natural History in Washington, D.C. before beginning graduate study in the Department of Ecology and Evolution at State University of New York (SUNY) Stony Brook. In 2011, he received his Master of Arts from SUNY-Stony Brook for his work with Dr. Lev Ginzburg.

James's research interests center on mathematical and statistical applications to ecology and evolution. His Masters work focused on the relationship between metabolic rate, body mass, and dimensional scaling across a variety of vertebrate systems, a field that is often referred to as metabolic ecology. Upon arriving at Florida State University, he joined Dr. Dennis Slice's lab in order to purse his interest in Morphometric techniques and applications.

In his free time, James enjoys film, writing, hiking, and cooking.

Before David R. Witman arrived in Florida, he was a Mechanical Engineering undergraduate student at Clarkson University in Potsdam, New York. He completed the degree in May 2011 as a President's List scholar, then applied and was accepted to the Master's program in Computational Science. David's interests in Computational Fluid Dynamics, teaching and research led him to Scientific Computing.



While at Clarkson, David was active in tutoring and community service. He tutored others in Thermodynmics, Fluid Mechanics and Matlab, presented his research and posters at conferences and workshop, and held membership in several engineering organizations, including Pi Tau Sigma, the Mechanical **Engineering Honor** Society, and Tau Beta Pi.

### Nathan Daniel Crock

graduated in 2008 from St. Petersburg College with an Associate in Arts degree before completing the Bachelor of Science in Applied and Computational Mathematics in 2011 from FSU. Nathan began his affiliation with Scientific Computing while still an undergrad by initiating a project with Gordon Erlebacher involving scene registration from point clouds with multiple Kinects.

Since 2006, Nathan has tutored mathematics, providing assistance while at St. Pete College, the FSU Math Help Center, the FSU Athletics Department, the FSU College of Medicine, and in private sessions. When he is not busy with coursework, Nathan spends time traveling



across the country, serving as president of the Renegade Boxing Club and the Anhelo Argentine Tango Club, and maintaining his website, mathnathan. com.

Ph.D. student Alisha Ciara Rossi comes to Scientific Computing after completing her BS in Biology from Milliken University in May 2003 and the Professional Science Master's in Computational Bioscience from Arizona State University in May 2006. Following the completion of her Master's, Alisha taught at the School of Interdisciplinary Studies and served as Coordinator of Math and Science mentoring for the University College at Arizona State University. She was the instructor for a variety of courses, including General Biology Lecture and Laboratory at Estrella Mountain Community College; Intermediate Algebra and Trigonometry at Glendale Community College; and College Mathematics and Plant **Biology at Arizona State** University.

#### Alisha is working with



Alan Lemmon on the development of novel statistical and computational approaches to areas of evolution including phylogenetics, phylogeography, speciation, population genetics, and genomics.

Feifei Xu received her undergraduate degree in Applied Mathematics in July 2011 from Fudan 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. 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.

New Students continued from page 7

University in Shanghai, China. While at Fudan, Feifei was recognized in the People's Scholarship of Fudan University, the China Undergraduate Mathematical Contest in Modeling, and the National Creation and Invention Contest. She programs in C++ and MatLab, and is interested in computational mathematics, biological science and biochemistry.

Feifei has done a wide variety of volunteering. She has contributed her time to the Ninxin League, an organization that teaches sign language; the Shanghai Science and Technology Museum; and the Youth Task Force of Zhide College at Fudan University.

Before coming to Scientific Computing, Feifei interned as an Assistant Manager of Marketing for Zhilong Industrial Development Incorporated, and as a statistician and surveyor for Qishou Consulting.



Wang's EWCVT continued from page 2

In EWCVT, algorithms developed to implement the model subdivide like segments of the image into clusters, then compute the boundaries of objects. Some of these algorithms are similar to the classic CVT model, but contain enhanced features, and allow computational economy.

A continuation, extension and enhancement of the EWCVT is the Local Variation and Edge Weighted Centroidal Voronoi Tessellation (LVEWCVT). The critical variable of this model is that it defines and calculates the centroids locally for each pixel, thereby increasing accuracy in images with high color variation.

In the two short years since the publication of EWCVT, Wang's work has been cited many times, and his image segmentation method has been applied in areas such as curve smoothing to assist in identifying important data patterns while excluding data noise. Scholars have extended and improved the EW-CVT method, and built on Wang's research. "As a simple, effective method in image segmentation, we can expect more research and other applications in this direction."