SC faculty named Developing Scholar

Scientific Computing

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Department

of



Sabbatical research & collaboration



Recent grad accepts position



Alum on postdoc @ Hopkins



Associate Professor Alan Lemmon was selected to receive the Developing Scholar Award, Florida State University's premiere award for faculty who demonstrate the greatest levels of promise for scholarly research. Lemmon was honored for his scholarly achievements at the 2017 Faculty Awards ceremony and dinner, an annual event held to mark the highest achievements of FSU's 2400+ faculty across all schools, departments, and divisions. Lemmon is an international expert in the field of bioinformatics, genomics, population genomics and biogeography, and was tapped for the award for his research and scholarly advances in the evolving field of phylogenetics.

Lemmon and Emily Moriarty [research collaborator and co-developer] have



Associate Professor Alan Lemmon

moved forward long-standing problems in the field of statistical phylogenetics through a process called Anchored Phylogenomics. With the introduction of complete genomic sequencing in the 1990s came added complications, including limited methods to parse the massive data that results from genome sequencing, and gene selection appropriate for the specific research. Lemmon and Moriarty developed an enrichment protocol that takes known data and uses it as a reference to target the genome of the desired species; they have found solutions to the initial choice of genes to target, to the problem of enrichment protocol, and to developing the complete pipeline of software to analyze the extracted DNA.

In nominating Lemmon for the award, Department of Scientific Computing Chair Gordon Erlebacher praised Lemmon's many laudable accomplishments in evaluation of species relationships and in improving the accuracy and precision of phylogentic research by developing new methods of data collection and analysis. "As a result of Alan's novel research methods, there has been a two orders of magnitude increase in performance and a two orders of magnitude decrease in the cost of genomic sequencing of phylogenetic taxa. This has revolutionized the field, causing scholars and corporations throughout the world to seek him out for collaboration."

continued, see Lemmon, p7

Slice sabbatical semester ends with collaboration

Dennis E. Slice, Scientific Computing professor and resident morphometrician, was approved for sabbatical leave to implement major functionality enhancements to his morphometrics (shape analysis) software. The sabbatical also included an international research collaboration and outreach component with universities in Europe and Africa, including the University of Vienna [where Slice holds an Honorarprofessorship in the Department of Anthropology] and the University of Witwatersrand in Johannesburg. The sabbatical semester is designed to provide opportunities for study, research, creative effort, teaching innovation, and related travel, all to enhance the quality of the recipient's service to the university.

"The sabbatical leave afforded me the opportunity to travel, work, and collaborate internationally to an extent that simply would

not have been possible while working around the normal semester obligations."

Slice used his sabbatical leave to teach courses in Geometric Morphometrics and Computational Forensics at the University of Vienna, Austria, where he worked with local faculty and helped students with their Doctoral

and Master's research. During his time there, he also developed a fifteenpart software tutorial on graphics programming in the Java language using OpenGL (via JOGL) and the OpenGL Shading Language. This open-source tutorial will be released shortly and available for download from the FSU Scientific Computing Morhometrics Lab (http://morphlab. sc.fsu.edu/).

Routines created as part of the above project are being incorporated into a newly developed library to extend and enhance the two- and three-dimensional graphics capabilities of Morpheus et al., one of the leading software packages available for shape analysis. Morpheus et al. contains sophisticated multi-dimensional analyses and graphics



Slice [rear center] with morphometrics workshop participants.

renderings, support for missing data, and batch processing; these features allow users to undertake complex analyses not explicitly hard-coded into the program. Once the new features have been incorporated and tested, a new version of the software will be released with full open-source code

"The sabbatical leave afforded me the opportunity to travel, work, and collaborate internationally to an extent that simply would not have been possible while working around the normal semester obligations." --- DENNIS SLICE

and documentation from the Morphometrics Lab website.

For the second part of Slice's sabbatical, he envisioned international research collaboration and outreach in Europe, but extended that to a second continent – Africa – with his association and alliance with the University of Witwatersrand. Slice's visit was sponsored by a grant to Dr.

Scientific Computing professor chief journal editor



Professor Anke Meyer-Baese

Dr. Anke Meyer-Baese, scientific computing professor served as chief editor for a special issue of Frontiers in Computational Neuroscience. The special issue is entirely dedicated to the topic, Advanced graph theoretical approaches in neuroimaging of neurodegenerative disorders. Topics for Frontiers journals are broad based, and include science, health, engineering, humanities, and social sciences.

Often, neurodegenerative diseases present as brain connectivity disorders which have neural structure and functional architecture that is poorly understood. This special issue of Frontiers in Computational Neuroscience introduced new computational science quantitative methods to learn more about neurodegenerative biomarkers and how these diseases emerge and progress.

As chief editor, Meyer-Baese led and coordinated the editorial process; she was assisted by three co-editors: Juan Manual Gorriz and Javier Ramirez from the University of Granada, Spain, and Claudia Plant from the Helmholtz Zentrum Munchen in Germany, a research center responsible for studying environmental health issues. Sixtythree authors from over the globe contributed to the journal.

See more at the Frontiers website, www.frontiersin.org.

Nanette Briers of the School of Anatomical Sciences in the Medical School of the University of the Witwatersrand with support from the head of the school, Professor Maryna Steyn. Local arrangements and hosting were done by Dr. Lynne Schepartz, also of the School of Anatomical Sciences.

At Wits, Slice lectured on "The Future of Applied Shape Analysis" and gave a workshop to students and faculty from Wits and other universities, including participants from as far away as California, on new and existing methods of general shape analysis using software developed and distributed by the Morphometrics Lab, Morpheus et al. and GPSA. He gave another workshop on morphometric methods for computational forensics featuring software developed in collaboration with Ann Ross of N.C. State University, 3D-ID (http:// www.3d-id.org/), and software produced as part of a current project funded by the National Institute of Justice, forAge, developed with fellow FSU faculty member Bridget Algee-Hewitt (Anthropology) and post-docs Detelina Stoyanova and Jieun Kim (Scientific Computing). All software is available from the Morphometrics Lab website except 3D-ID, which has its own site.

Both workshops were well-received and the faculty and students in attendance were eager to contribute to both forensics projects, 3D-ID and forAge, by testing methods and digitizing new data from the unique and extensive collections in South Africa.

"The South Africa visit was an opportunity that presented itself above and beyond what I had originally planned, but I am really glad I was able to take advantage of it. South Africa proved to be a fascinating place in its own right, and it was a great honor and opportunity to be able to connect, in person, with the outstanding faculty and students at Wits."

See more at the Morphometrics Lab website, morphlab.sc.fsu.edu.

Geshel lands position at Texas Instruments

When Christine Geshel went to Engineering Day back in September, she was hoping to find out more information about how the event worked and the companies that were there. Now she's headed to Texas this summer after accepting a position at Texas Instruments as a data analyst.

"This was my first time going to Engineering Day. I first heard about it through an email from the Career Center. They send information about Engineering Day to students in the science, technology, engineering and technical skills fields.

"After I received the email, I looked online at the companies recruiting at Engineering Day -- I was looking at companies who were interested in computer science or software engineering majors. Texas Instruments was attractive specifically because they are ranked in the top fifty places to work on glassdoor.com, and because there is a lot of room to grow and advance in their company."

On arriving at the Morgan Building, Geshel approached the

he said he would be interested in interviewing me in a few days because of my background. I then spoke to their HR representative who scheduled a behavioral interview two days later at the FAMU career center."

Once the interview was scheduled, Geshel began her preparation. She did research on behavioral interviews, and learned about their structure so she knew what kinds of questions to expect. Because behavioral interviews focus on how the candidate has handled past situations, it tends to be more predictive; Geshel used the time between Engineering Day and the interview to consider what types of skills and behaviors the company might desire, and to think about the best method to present her past experiences. Geshel was successful in the first interview, then had an additional interview via the web before flying to Dallas for the final meeting.

"I had three interviews with TI. During the first interview at FAMU's campus, Patrick, the CS/IT recruiter, performed

Geshel used the time to consider what types of skills and behaviors the company might desire, and to think about the best method to present her past experiences.

recruiting tables and made the rounds, talking to different companies about what positions they had available to see whether they matched her particular skills and career goals. "I approached Deloitte, IBM, Microsoft, Home Depot, Procter & Gamble and PepsiCo while I was there. I had researched companies who would be there, and based on that, thought these were the best companies to talk to.

When I approached the Texas Instruments booth, I introduced myself to one of the recruiters and discussed my major and interests; he then redirected me to another recruiter who was specific to computer science and IT students. I gave another brief introduction of myself and my interview. He asked questions about how I deal with stress, difficult people, and working in groups. The second interview was virtual. There were prerecorded questions on the website and I recorded video responses to the questions. I got a call a week later from an HR representative from Dallas. We figured out scheduling for when I could visit, and a few weeks later I flew out to Dallas.

"The first day we mostly just did networking and informational events. When I arrived, we were taken into a meeting which introduced different members of the company and told us more about the rotation program. Afterwards, we went to a networking event where I met people in the

Geshel displays her research at the department's annual research exposition

A Parameter Study of a Feed Forward Convolutional Neural Network Christine Geshel, Gordon Erlebacher, PhD Florida State University, Department of Scientific Computing	
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company and the various interviewers. Lastly, we went out to dinner with the HR team, and younger employees. The next day was for the interviews. There were two 45-minute interviews with three interviewers each. They asked me about problem solving and working with teams. They asked me technical details of things I had listed on my resume. Overall the experience really wasn't as stressful as I had originally thought."

Having been impressed by the company during the multistep interview process, Geshel accepted a position in the IT rotation programs in TI's Application Branch. "I think they were most impressed by my time management skills and my problem solving style. I knew the position was right for me because I could tell Texas Instruments cares a lot about their employees. Many people I met while in Dallas have been there for an upwards of 15 years and they all seemed really happy. I also liked that they promoted networking and meeting people outside your department. They have created a lot of groups within the company for new employees to meet new people which I think will help a lot with my transition to Dallas."

Geshel moves to Dallas and begins her new position this summer, and is excited about getting started. Already she has gotten positive feedback on one of the most important skills she'll need to master to be successful in the position. "They mentioned a couple of times that I seemed calm or at ease which they seemed to like. They mentioned it's a steep learning curve when you start, so initially time management and staying unstressed will be needed right away. Overall I think knowing how to work effectively with a team, and problem solving as a group will be important in the long run."

For more, go to www.ti.com & www.sc.fsu.edu.

Rios visits department

As soon as SC alum Fernando Rios returned to the department, his professor, Ming Ye, put him to work. "Excuse me," he says as a student stops by. "Ming asked me to hand back quizzes to his students. He had to go to a meeting outside the building."

Rios left Scientific Computing in 2010 after completing his Master of Computational Science degree. In 2015, he was awarded the Ph.D. in Geography from the University at Buffalo, SUNY; he works at the Johns Hopkins University main campus library. "Hopkins has several campuses - there's the metro campus - the medical school's there - which is downtown. I work at the Homewood campus which is the main campus. That's where they have the school of engineering, arts and sciences - everything that's not medical or business. That's where the library is as well."

Homewood's 140-acre campus, where most undergraduates study, is located in North Baltimore, prominently situated in the most heavily urbanized region of the U.S. Commuting, living and working in the northeast is radically different from the Tallahassee experience. "Physical access to your job is a premium because of driving time. A lot of people live downtown and don't even own a car. There's no parking, and the commute - I work with some people who actually live in Pennsylvania. Traffic can be really nightmarish! Sometimes I hear it takes two hours to go a very short distance - you could walk and get there faster. I live relatively close by, and I drive or bike to work."

Like many recent Ph.D. graduates, Rios found a limited time position as a postdoctoral associate immediately after graduation. His postdoc, though, is a bit different from most. Instead of working with a professor in a laboratory, Rios works for all faculty and staff as part of a data group housed at the George Peabody Library.

"I work in the data management services group. It's a unit attached to the library. We provide services to support researchers and all their data needs. We provide services around data management planning, data management training and best practices for working with data. An example of what we might provide is versioning services for your data or we might help provide identification if you're doing human subjects studies. We provide data archiving services; for instance, a researcher might come in, and they have to share their data because the funding agency says they have to share it. We might help them

with that by putting it on our data archive, or by helping them find an appropriate place to put it. So it's really a consulting and service unit, which makes my position pretty interesting as a postdoc. It's not a traditional position where you're working in a lab or for a professor on a grant funded project, which the vast majority of postdocs do. I have a lot of freedom to do what I want to do."

An additional aspect of Rios' work is consultation with faculty in creating and archiving research software. Over the years, Hopkins scholars have created software for courses and research projects that Rios is beginning to locate, review and catalog. Before these efforts, there was no place faculty and university researchers could go to find out what software exists and with what capability.



George Peabody Library at Johns Hopkins University. Photo by Matthew Petroff.



Scientific Computing alum Fernando Rios

"Now that I've been there a while, I'm looking at software that researchers create. Not data, but software. It's really a new kind of idea to provide services for supporting research software in terms of best practices, managing, archiving, preserving research software. They kind of had this thought that they need to look at these things, but they didn't know where to start. That's what I've been doing - researching what people have done and setting up scaffolding for them to start to integrate software into their workflows. It's really been an exploratory thing almost because nobody was doing this in this kind of service oriented setting."

Before accepting this position, Rios wasn't aware of the wealth of job prospects in academia, but outside the classroom. Because he enjoys the freedom and evironment of this position, he plans to pursue similar opportunities when this one concludes.

"I like academia, but being a professor is not really my cup of tea. I never really considered what possibilities there might be for staying in academia, and the libraries are a really good place to be. In fact, there are a lot of possibilities for people who are looking for alternative academic careers. There are positions in research administration, data management services and many other opportunities working with subject matter experts. I want to stay in this general area of work – that's my goal at the moment."

For more information and to see projects Rios worked on, go to: http://dms.data.jhu.edu/ https://twitter.com/riosfrnd http://fernandorios.net

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Lemmon, continued from p1

In addition to his research, Lemmon has contributed to collaborations, mentoring and teaching, publications, reviews, and community service. He has dedicated his time to develop and teach probe-design workshops to faculty, postdocs, and students, and he created an annual workshop to help students write and win grants. Lemmon teaches courses on a regular basis in Computational Science and a course on biology of animals that takes students out into the field for observation and data collection.

"Alan has an outstanding command of all aspects of computational phylogenetics, bioinformatics, the techniques of data science, and Bayesian statistics. He has managed to combine this knowledge to blend research, science and entrepreneurship, and researchers throughout the world are seeking to have him analyze data that leads to research ventures and new insights into the interrelationships between species on a vastly grander scale than previously possible. It is my belief that Anchored Phylogenomics is one of the key innovations for the student of genetic species relationships in this decade," said Erlebacher.

A Developing Scholar recipient receives a one-time award of \$10,000 that is to be used to promote the awardee's program of research and creativity during the academic year following the award's presentation. Selected candidates are mid-academic career faculty with a strong cumulative record of achievements in teaching, service, and research.

For more, go to http://anchoredphylogeny.com/ https://www.research.fsu.edu/research-offices/opd/crc/ programs/dsa/ www.sc.fsu.edu Department of Scientific Computing 400 Dirac Science Library P. O. Box 3064120 Tallahassee, FL 32306-4120 www.sc.fsu.edu

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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 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.

Our Computational Exposition this year was one of the best ever! To see more research and video footage go to our FACEBOOK page at www.facebook.com/FSUSciComp.







From left to right:

* Research by Eitan Lees: How the presence of cracks or long channels in porous media lead to anomalous diffusion.

- * Research by Hongzhuan Lei: Plume of ammonium concentration.
- * Research by Benjamin Crysup: The error in the relative density of coarse grained particles of neopentane using various course-graining methods.

