Fall 2017

Department of Scientific Computing

Slice delivers Rohlf Medal keynote

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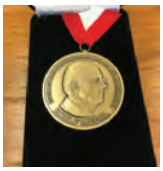
Professor Dennis Slice, this year's recipient of the Rohlf Medal for Excellence in Morphometric Methods and Applications, was honored at his alma mater, Stony Brook, with Slice giving the keynote at the Provost's Lecture Series. Slice's presentation was entitled, "An Unexpected Journey: A Curious Career in Shape Analysis." Presented every two years to distinguished members of the morphometrics community, the Rohlf Medal is bestowed for outstanding work on the development of new morphometric methods or applications in biomedical sciences.

While at Stony Brook, Slice studied and worked as a research assistant under the supervision of James Rohlf, for whom the award is named. Following graduation and a postdoc, Slice took on teaching, administrative, managerial and consultation roles before returning to university research and teaching at Wake Forest University School of Medicine. Slice joined the faculty at the Department of Scientific Computing in 2008, and has sustained an affiliation with the University of Vienna where he has been Honoraprofessor in the Department of Anthropology since 2000.



Slice's most notable work is in the field of shape analysis, which can be used in applications as diverse as forensic investigations or the fit and function of protective equipment (respirators & head gear). Slice is known among his peers as a leader in morphometric data analysis and statistical computing, skeletal analysis, and shape estimation.

Slice is the first and only Stony Brook alum to win the Rohlf Medal for Excellence.

To watch a video presentation of Slice's keynote, go to https://www.youtube.com/watch?v=DqxFfXDyFC4&t=0s

For more info about Slice and his award, go to http://news.fsu.edu/news/faculty-staff-briefs/2017/11/17/faculty-staff-briefs-november-2017/

For more on Slice and the Morphometrics Lab at FSU, go to: http://morphlab.sc.fsu.edu

Slice looks on as the Rohlf Medal for Excellence keynote presentation is rebroadcast .

Sockwell to research climate at national laboratory

Doctoral candidate Chad Sockwell is a recipient of the Science Graduate Student Research (SCGSR) program award from the U.S. Department of Energy, a highly competitive national award sponsored through the DOE's Office of Science. Sockwell will spend a year – January 8, 2018 – January 7, 2019 – working on a research project with the use of lab equipment, facilities, expert consultation and other resources provided by the Los Alamos National Laboratory (LANL).

Department of Energy SCGSR award recipient, Chad Sockwell

"I applied after Max [Gunzburger] sent me an email and encouraged me to apply. I think the labs want to interact with the best people. The DOE seems to be interested in mining the universities for people who are working on interesting research and are a good fit, so they try to get people in the door by investing in them with awards and fellowships," said Sockwell.

Sockwell's research proposal, Algorithmic Improvements of the Temporal Scheme in the MPAS-O Software for Multi-Resolution Climate Modeling, was of interest to Dr. Todd Ringler, scientist and climate modeling expert in the Theoretical Division at LANL. Dr. Ringler will be Sockwell's mentor for the year, with research support and collaboration provided by his advisor, Max Gunzburger.

"This program is extremely competitive, so it's quite a coup for Chad to get the award. I should add that it is also impressive that Dr. Ringler, who is going to be his mentor at LANL, is the leader of the team that is developing the ocean component of the new DOE Earth System Model so that Chad's work at LANL will not only be of importance to the computational science community, but will also have immediate impact on the next generation of ocean models," said Gunzburger.

> ".....Chad's work at LANL will not only be of importance to the computational science community, but will also have immediate impact on the next generation of ocean models."
>
> --- MAX GUNZBURGER

Department Chair Gordon Erlebacher adds, "Computational science is greatly impacting many fields of research and our students are at the forefront of this wave. Chad's research lies at the intersection of mathematics, numerical analysis, and climate science. If he is successful, climate models will run much more efficiently, greatly enhancing the number of climate studies possible on existing hardware, with commensurate societal impact."

"I'm working to develop exponential integrators as my research project. What we are trying to do is increase the amount of information we can learn from climate models by removing model restrictions and increasing time steps. For example, gravity waves give us a restriction, and we don't care about resolving them exactly, except to remove the restriction. If we can do that, we can simulate at larger time steps. For climate change, we care about large time

see Sockwell, page 4

Nason puts computational skills to work

When undergrad student Livia Nason decided to get the bulk of her coursework done as early as possible and learn as much as she could about problem solving and programming, she was simply using her time efficiently.

After doing a directed individual study in the spring term, she was looking to get her hands dirty – at least in the computational sense. "I learned Python through this department in the Programming for Scientific Applications course. I had also just learned R in the spring in Computer Applications in Psychology, and in the same semester, I had taken the Geographic Information Systems course and learned about GIS. By the time the summer came around, I was all set up to work at the FGS."

On a tip from a professor this past summer, Nason applied for a job to work with the Florida Geological Survey; she found out about the position from Professor Ming Ye, after completing some related coursework. "I did a DIS with him last spring. The DIS involved reading scientific papers about water quality and transport and then presenting them to other students in the seminar. I learned a lot in that class, mostly about how to study papers and present them, but it also acted as an introduction to real world water quality issues, and how both geology and human activity play important roles in those issues."

"After the DIS, I was looking to participate in an internship for the summer. It was around the last week of the semester when Professor Ye suggested that I look into the FGS and talk to them about their internship program. We found an application packet online and I filled it out. I went to the FGS with my resume, sat down with the program coordinator, and immediately got an internship for the summer. It was very last minute, but I'm so glad it happened."

Because Nason is majoring in Computational Science and has progressed so far in her coursework, her internship experience is different from that of the typical FGS intern. The programming skills Nason learned in the major made her an attractive candidate for higher level work – work outside the scope of what most interns do for the organization.

"Most FGS interns essentially organize books and data and make sure the data in the computer matches the books. But when I arrived, one of the staff, Seth Bassett, saw my resume and said, 'Oh! She's a programmer! I want her to be my intern!' He's the programmer in the office and he works primarily in R and Python on GIS data. When he saw that I was familiar with these languages, he wanted me to work with him and has been mentoring and teaching me about his projects. Unlike some of the previous computing interns, I have learned to love the work that I do, and that's exactly why I'm here, to do this particular kind of work."

Livia Nason

Nason works on the STATEMAP Project (SMP), a study of Florida's geology; the project is essentially a study of the history of Florida's topography. The SMP is a systematic study of the state – usually focusing on two or three counties at once – in which scientists study the geology in a particular area. The goal is to map the geology of the entire state.

see Nason, page 4

Sockwell, continued from page 2

steps – things like global ocean circulation, temperature changes – these occur at a much larger, slower time scale. That's really what we want to simulate accurately, and if we simulate at the time scale of the gravity waves, this slows down the research. We want to skip over the gravity wave simulation and concentrate on all these other, slower time scales, so that's what we're working on.

"In doing this research, I work closely with Konstantin Pieper who is a postdoctoral associate in the department. He has a very broad and deep knowledge of mathematical analysis, whereas I have a stronger background in physics and computational science, and I speak to him daily. I have the best of both worlds with Max and Konstantin. It's sort of like I have a very wise mentor who helps me realize the big picture and the future of my career, and then I have a second colleague who is very hands on and I interact with almost daily."

Currently, Sockwell is feverishly preparing to close out the semester and get packed for the move. He still has school work to finish, and needs to get everything ready for the trip to New Mexico.

"I found a place to rent on craigslist that's about 30-40 minutes northeast of Los Alamos in a small town right outside of Alcalde called Los Luceros. I used to live in a small town called Hosford, which is a little ways out of town from Tallahassee, so the drive will probably be about the same as it was when I lived in Hosford. My girlfriend, my dog and I are packing up and leaving right after Christmas."

Sockwell is one of 52 awardees for 2017 from universities across the nation. The award pays a monthly stipend of $3000, and provides resources for travel. The SCGSR program prepares graduate students for careers in STEM fields that are important to the Department of Energy's mission. The award provides supplemental awards to outstanding United States graduate students to pursue part of their graduate thesis research at one of DOE's twelve national laboratories in areas that address scientific challenges central to the Office of Science mission. This opportunity advances the students' doctoral thesis while providing access to expert mentorship, outstanding computing facilities and other resources available at national labs.

See more at https://science.energy.gov/wdts/scgsr/.

Nason, continued from page 3

"First, the geologists go out into the field with drilling trucks, where they drill boreholes and take a core sample of rock. Throughout Earth's history, different types of sediments collect on an area and the core sample gives scientists a slice of this history in rock form. Geologists look at the rock samples and analyze them – they classify the rock by the type of sediment and record the depth at which it was found, then they input the information into a database. This information can tell us about the locations of important minerals, as well as details about past climates and environmental conditions – the history of Florida is in those samples."

Nason's primary work at the FGS is to confirm data quality and data control. When she receives new data, she works to develop different methods of discovering errors within the extensive dataset. Errors can come in many different forms including incorrect sample depths, incorrect borehole locations, or incorrect sediment classifications, which all stem from simple human error. Because of the various types of datasets and errors, Nason must formulate new algorithms that are used to identify them. Once she has found a possible data error, she discusses it further with her mentors and they determine how to proceed based on their best knowledge.

Above: 94ft core taken in Levy County

Because Nason took so much coursework before her senior year, she has a light load this term, and is continuing her work through this academic year at the FGS. "We just finished working on STATEMAP in the St. Petersburg/Tampa Bay area last summer, and we are going to start working on Kissimmee this year. In the fall, I worked about ten hours a week on top of my class schedule, but I plan to devote more time to the FGS in the spring since I will only be taking the Senior Practicum. I am thankful that the Department of Scientific Computing has prepared me so well to work with and manipulate data; and because of that, I am qualified to be in this position."

See more at the Florida Geological Survey website, https://floridadep.gov/fgs.

New students, staff at SC

Siddhartha Bishnu

Ezra Booker

Michelle Claycomb

Karey Fowler

Although Siddhartha Bishnu is a doctoral student in Computational Science, he is jointly enrolled in Earth, Ocean & Atmospheric Science for the fall semester. Bishnu has been a graduate student at FSU since 2012, having received an MS in Applied and Computational Mathematics (Summer 2016) and will graduate with a second masters in Physical Oceanography in December after completing and defending his thesis. Originally from Kolkata, India, Bishnu completed his undergraduate degree at the Indian Institute of Technology (IIT) in Kharagpur before coming to Tallahassee for his graduate education.

In his spare time, Bishnu enjoys spending time with friends, reading novels, and watching movies and television series at home. When time permits, Bishnu, a former competitive powerlifter, sketches and paints.

Bishnu plans to study numerical ocean modeling with Bryan Quaife, Max Gunzburger and Mark Peterson, a researcher at Los Alamos National Laboratory.

New grad student Ezra Booker is from Lake City, Florida, just 90 minutes east of Tallahassee. While an FSU undergrad, Booker worked with David Collins to analyze simulation data of star-forming collapsing molecular gas clouds. This research project was concerned with the mean magnetic field strength (Bmean) simulated in the gas cloud and how variations in the Bmean affected the star formation rate in the simulation. The goal was to answer one more piece of the puzzle of why the observed stellar formation rate does not match the theoretical rate. Booker graduated with dual BS degrees in physics and astrophysics in 2015.

For his graduate research, Booker plans to work with Tomasz Plewa, and is in the beginning stages of a possible thesis project centered on further investigating double white dwarf star merger models developed by Plewa and his former student Daniel Fenn.

Booker enjoys spending time with fellow students on the weekends, and is a practiced musician. He plays guitar, bass guitar, and trumpet and is developing his singing skills. He enjoys reading and building effects pedals for guitars and bass guitars.

Michelle Claycomb joined the department in May 2017 to handle travel, purchasing and human resources duties. She is from Miami, originally coming to Tallahassee for school. She has an undergraduate degree in English Literature, and a Master of Library and Information Studies, both from Florida State.

Before coming to the department, Claycomb worked as administrative assistant at the Center for Intensive English Studies, the university's resource that helps students increase English language proficiency. She also worked as a bookkeeper at McAlpin, Cavalcanti & Lewis, a CPA firm in Okeechobee, Florida.

Claycomb is single, and mother to a daughter, Penelope. Her hobbies include cycling, photography and crafts.

Karey Fowler is the new Academic Advisor for the department. Fowler is a pianist; she received B.M. and M.M. degrees in Piano Performance from FSU and the University of Massachusetts, Amherst, respectively.

After graduating from FSU, Fowler and her husband lived in Austria where she studied music and taught piano at the

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Ashley Gannon

Brandon Gusto

Marzieh Khodaei Gheshlagh

Kevin Mueller

American International School in Vienna. On returning to the states, she worked for a time as a musician at the Creative Dance Company in Birmingham; she left Alabama to accept a faculty position in dance at UMass, and to teach courses in music appreciation and rhythmic analysis.

Prior to working for the Department, Fowler was a paralegal for Legal Services of North Florida. For seventeen years, she was the academic advisor at FSU's College of Music.

Fowler is the organist at Fellowship Presbyterian Church, and continues private piano studies with Dr. Read Gainsford, Coordinator of Keyboard Studies at FSU's College of Music. She has a son, Christopher. If you would like to hear her play, go to http://www.fellowshippc.org/music-archives.html.

Ashley Gannon comes to Scientific Computing after graduating from FSU with two undergraduate degrees – one in Biological Sciences, the other in Biomedical Engineering. Gannon is a Florida native from Loxahatchee, an unincorporated community in Palm Beach County near West Palm Beach.

As an undergrad, she worked for two and a half years with the Center for Brain Repair in the Department of Biomedical Sciences. There, Gannon helped create a mouse model for attention deficit hyperactive disorder (ADHD). The group's research made the crucial connection that hyperactivity and working memory deficits are associated with two specific types of dopamine receptors. Gannon's group also studied the role of dopamine in other mental health disorders, including Parkinson's and schizophrenia, an area she would like to study further. She plans to work with Bryan Quaife to create a model for dopamine reuptake by modifying his vesicle separation models.
In her leisure time, Gannon enjoys playing chess and word games, reading about medical advancements, and baking. She also volunteers for a couple of local animal rescues, and has fostered many cats.

Brandon Gusto began studying at FSU in 2013 as a mechanical engineering student, and soon found so much pleasure in the required mathematics courses, he declared a second major in applied and computational mathematics. His curiosity extends to computational fluid dynamics, aerospace vehicles and technology as well. As an undergrad, Gusto began working with Kunihiko Taira in the mechanical engineering department on a theoretical fluid dynamics project, solving for the initial flow field of an impulsively started cylinder. Gusto then moved on to other projects, including a computational simulation of the flow around a circular cylinder using commercial LES software. He worked with Wei Guo at the National High Magnetic Field Laboratory where he developed statistical analysis code for the post-processing of data obtained from a cryogenic liquid helium experiment. Gusto was then offered and accepted a fellowship to attend the Los Alamos National Laboratory Computational Physics Student Summer Workshop where he worked on parallelization techniques for LANL's newest 3D shock hydrodynamics solver called Chicoma.

Gusto decided to stay at FSU to pursue the Ph.D. because of the faculty relationships he has developed over the years. Although his research topic is not completely decided, Gusto plans to study the development of wavelet-based numerical fluid dynamics solvers for a variety of flow regimes and will work with Gordon Erlebacher and Yousuff Hussaini.

In his limited free time, Gusto enjoys exploring and finding exciting things to do in Tallahassee with his girlfriend, Marie; they both enjoy an active lifestyle which includes working out at the gym and jogging regularly.

Doctoral student Marzieh Khodaei Gheshlagh received the Bachelor of Science degree in pure mathematics in July, 2005 from Mohaghegh Ardebili University in Ardabil, Iran. She received the Master of Science degree in applied mathematics three years later (December, 2008) from the University of Tehran.

During her academic career, Khodaei Gheshlagh has been an active researcher, presenter and lecturer. She has presented papers at international conferences in operations research, and has published her work on network flows in the International Journal of Mathematics in Operational Research. Her other research interests include operations research, optimization, network flows, linear programming, graph theory, and theoretical computer science.

While in Iran, Khodaei Gheshlagh lectured to degree program students at the associate's and bachelor's levels in operations research, general and applied mathematics, math for computer science, statistics, probability inferential statistics, computer basics, information & communications technology and electronic services.

When she has time, she enjoys painting, poetry, photography, cycling, mountain climbing, swimming, tennis and chess.

Kevin Mueller came to Tallahassee from Mobile, Alabama, having graduated with the bachelor of engineering degree in Electrical Engineering from Auburn University in 2014. After graduation at Auburn, Mueller attended graduate school and took his masters at the University of Washington where he studied applied mathematics. While completing his MS, Mueller worked as a junior data scientist at a start-up company now known as Jobalign. While at Jobalign, he worked with speech emotion recognition, or more specifically, the process of trying to automatically predict a user's emotions from speech data.

Mueller's research interests lie in optimization, artificial intelligence and machine learning. Currently, he is working with Gordon Erlebacher to help build a new deep learning course. In his leisure time, he enjoys playing video games, mobile development, and hiking.

Marcelina Nagales is a Scientific Computing alumnae, having graduated with an undergraduate degree in Computational Science in Summer, 2017. She is currently the manager of the Morphometrics Lab in addition to being a doctoral student in Computational Science with a focus in anthropology.

Marcelina Nagales

Nagales found her passion for computational anthropology while working with SC Professor Dennis Slice (see related story, page 1) and Alexa Pennavaria, a fellow student who graduated in Spring 2016. She has contributed to a research project focused on scanning archaeological projectile points/knives and constructing a database of typologies. Currently, she is working on another project with Chase Van Tilburg, an undergraduate in the FSU Art History department, for the purpose of digitizing the John House Stereograph Collection and further

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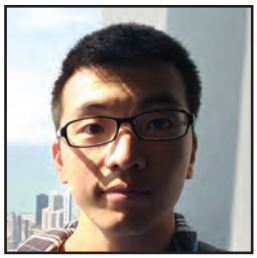
George Owen



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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.

enhancing the digital museum experience. She continues to pursue her research in the Morphometrics Lab by analyzing different types of laser scanner methodologies.

Her current interests outside of school include writing poetry and reading science fiction. She also enjoys stand up paddle boarding and playing recreational soccer.

Originally from Nashville, Tennessee, George Owen attended Louisiana State University in Baton Rouge for his undergrad studies, receiving the bachelor of science degree in mathematics with a focus in computational mathematics, as well as minors in economics and history. In the summer of 2016, Owen participated in the summer REU Program for High Performance Computing at the University of Maryland, Baltimore County. While there, he participated in performance testing on the new generation of Intel Xeon Phi processors known as Knight's Landing.
Still undecided on his research path, Owen is broadly considering the study of machine learning. Currently, he works with Xiaoqiang Wang; the two are developing a parallel programming class for next semester.

Owen enjoys the study of history as a pastime, and loves to listen to history podcasts. His favorite podcast is The History of Rome by Mike Duncan, which covers the entire history of Rome from the founding of the city in 753 BC to the last Western emperor in 476 AD. Owen is also a self-declared football junkie and watches every game he possibly can on Saturdays.

sc.fsu.edu

Jingze Zhang completed his undergraduate studies in mechanical engineering at the Beijing University of Aeronautics and Astronautics, receiving the bachelor of science degree in 2017. Zhang's undergraduate research projects included the application of SVM and neural networks on mechanical processing. In addition, he has experience and interest in transfer learning, machine learning and data mining.

When he has time, Zhang enjoys swimming, badminton and ping pong, and he enjoys electronic music. He is looking forward to making new friends and travelling while in the U.S. pursuing his graduate degree.