Fall 2018

Department of Scientific Computing

CONTENTS

Plewa's research introduces new supernova model

Scientists have studied fusion, supernovae, and the Rayleigh-Taylor instability for more than a century in the quest for clean, inexhaustible sources of energy. Fission, the current method of energy production, involves dividing one atom into two, whereas fusion combines two atoms into one. Fusion takes place naturally in stars at extreme temperatures and enormous gravitational pressures. Scientific Computing Professor Tomasz Plewa studies nuclear fusion and supernovae; he and colleagues recently published research in the journal Nature Communications which changes the model for nuclear fusion.

"In principle, fusion is a never-ending source of energy as the fuel can be produced using a fraction of the energy produced in the process," said Plewa. "Currently we use fission which is exploited in nuclear power plants. Fission relies on access to radioactive ore, which has to be mined and prepared before it is utilized. These processes create safety and environmental concerns."

"Rayleigh-Taylor is a type of fluid instability in which one fluid tries to slow down the motion of a faster fluid. The process is susceptible to small perturbations at the interface separating the fluids, which grow very rapidly in time and leads to fluid mixing. If the fluids are thermally conducting, e.g. ionized gases (plasma), diffusion of heat will occur and modify (reduce) the instability growth."

Until Plewa and colleagues' latest research, models of nuclear fusion - reactions constantly underway in the core of stars – omitted how heat-causing energy fluxes impact the mixing of liquids, gases or plasmas. These processes are difficult to model; as they occur in stars, there is no way to observe them in real time.

Professor Tomasz Plewa

"We proposed a new type of laser experiment in this paper. Such experiments are expensive and require detailed modeling and computer simulations before a decision is made to field them (actually execute at some laser facility). This includes not only driving the flow using high power lasers but also proposing the optimal diagnostic system configuration."

To study the effect of heat in supernovae remnants, the research team turned to NIF, the National Ignition Facility, to model and perform the experiments. The team found that increased energy fluxes and their resulting heating reduces Rayleigh-Taylor instability significantly - by approximately 30% - and this reduction may increase over time.

"Supernova experiments typically included some density variation, possibly a material interface, which is subjected to strong forces. The paper discusses the surface of the star which separates its dense interior from much less dense stellar wind. Two materials of differing densities are used to represent that structure in the experiments.

continued, see Plewa, p. 3

Courses use contemporary topics & approaches

Mendoza-Cortes introduces new course on machine learning & quantum computing

Jose Mendoza-Cortes is preparing students for the world they will inhabit in the coming twenty-plus years, a time when an ample population of jobs will disappear, and others – jobs that require more specialized, sophisticated skills – will be the norm. Some who are striving to invent and design this new era are calling it the Fourth Industrial Revolution, a time where technologies bring together physical and virtual worlds, disrupting manufacturing processes, changing the way data is analyzed, and altering how the world consumes goods, and services.

Mendoza-Cortes sees his course as an opportunity to give students a broad foundation for the approaching changes computing will bring to industry. "At the conclusion of the course, my goal is for students to have a broad understanding of machine learning, data mining, and statistical pattern recognition, and grasp quantum computing at the first approximation," Mendoza-Cortes said.

To that end, Mendoza-Cortes has included a wide variety of machine learning and quantum computing topics in the 2-credit hour course. Students are learning the most effective machine learning techniques, the theoretical underpinnings of different machine learning - artificial intelligence, and the practical skills needed to quickly and powerfully apply these techniques to new problems.

"Machine learning is the science of getting computers to act without being explicitly programmed. In the past decade, machine learning has given us self-driving cars, practical speech recognition, effective web search, and a vastly improved understanding of the human genome."

In the quantum computing portion of the course, Mendoza-Cortes focuses on topics that pair quantum computing with computation heavy, sophisticated tasks. Quantum generative adversarial learning, for example, uses qubits - the quantum answer to binary's zeros and ones - to discriminate between real data and false, computer generated data. Other topics the course covers: (i) Supervised learning (parametric/nonparametric algorithms, support vector machines, kernels, neural networks). (ii) Unsupervised learning (clustering, dimensionality reduction, recommender systems, deep learning). (iii) Best practices in machine learning (bias/variance theory; innovation process in machine learning and AI). The course will also draw from numerous case studies and applications, so that students learn how to apply learning algorithms to building text understanding (web search, anti-spam), computer vision, medical informatics, audio, database mining, and other areas. (iv) implementing the first quantum algorithms in a quantum computer simulator.

Students bring their laptops to use during class; out-of-class work requires Python, MATLAB or Jupyter, all of which are provided through departmental computing resources. Machine Learning & Quantum Computing is taught on Friday from 2-3pm in 499 Dirac, the Seminar Room. The course is not intended to be math-heavy at the beginning, and is for anyone interested in machine learning and quantum computing.

The initial course has been successful, and Mendez-Cortes plans to expand the offering to two courses in the coming semester (Spring 2019). The first course, Machine Learning for Science and Engineering, is 3 credit hours. The second is two credit hours and is entitled Introduction to Quantum Computing: Theory and Practice.

For more on these courses, go to: http://mendoza.eng.fsu.edu.

Computational Thinking course available online

Professor Janet Peterson has developed the department's first online course, Computational Thinking, to begin in Spring 2019. The course has been given in the standard face-to-face format since Spring Semester 2017. This introductory course considers the question of how computers have come to imitate many kinds of human intelligence by detecting patterns in nature and by mimicking

patterns in the way humans interpret and process information.

Preparation for the course has been underway since January 2018; the first steps for Peterson were to make contact with the Office of Distance Learning and meet with representatives to discuss her approach and timeline.

"I contacted ODL to talk with them about the differences in structuring a course online as opposed to one that is taught in person. They gave me advice about course goals, activities and assessment methods for an online environment. One of the things that stood out from that meeting is that presenting material online has to be packaged differently than in the classroom. For an online course, it's important to create many small, complete capsules of information. That way, the student can easily understand each concept, and review those they need to repeat."

Computational Thinking satisfies three of six semester hours required to fulfill the university's Liberal Studies Quantitative and Logical Thinking course requirement. The quantitative and logical thinking courses are designed to help students become critical analysts of quantitative and logical claims by applying appropriate methods to solve real-world problems and by using a variety of ways to represent problems and solutions.

For more about Professor Peterson and the Computational Thinking course, go to: https://canvas.fsu.edu/
For more on the Office of Distance Learning, go to: https://distance.fsu.edu.
For general information on university liberal studies course requirements, go to: http://liberalstudies.fsu.edu/curriculum.html.

Plewa, continued from p.1

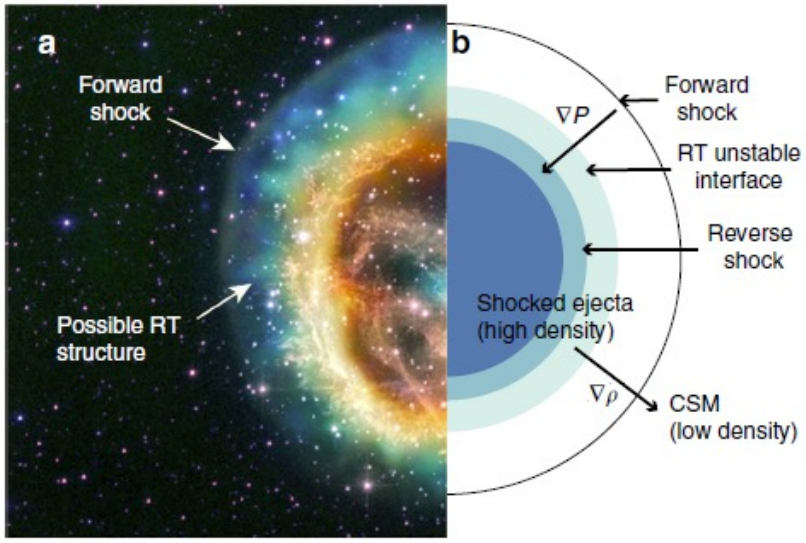


Image of supernova remnant. a False-color image of SNR E0102.2-72. This object is believed to result from a core-collapse supernova about 1000 years ago. One can see the edge of the forward shock. The modulated boundary within it might be structuring of the ejecta-CSM interface produced by RT. The brighter, inner colors are attributed to emission from the higher-Z, interior portions of the ejecta. The authors credit John Hughes of Rutgers University with having called the potential connection to RT to our attention. Image credit: X-ray (NASA/CXC/MIT/D. Dewey et al. and NASA/CXC/SAO/J. DePasquale); Optical (NASA/STScI). b Schematic (size and shape not to scale) of inner structures of the supernova that creates the opposing density and pressure gradients to create an RT unstable interface.

"Mixing between two fluids is not always practical or desirable. For example, fuel and oxidizers must be well mixed in combustion engines, cars and rockets alike. In the case of fusion, however, fuel is self-burning (so to speak) and one wants to keep it under uniform conditions at all times. If density gradients are present, fluid mixing will occur (typically due to Rayleigh-Taylor instability growth) and lower the burning efficiency."

The technology for fusion reactors is not quite ready, but continues to develop. One prototype reactor, ITER, is under construction in France, and experiments with another fusion process are ongoing at Livermore. The two facilities will use different equipment and methods (magnetic confinement v. inertial confinement) to perform fusion experiments.

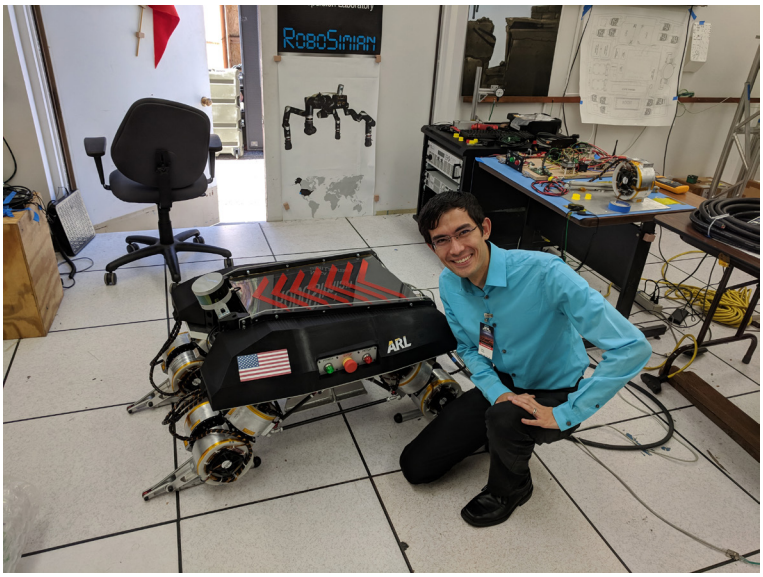
For more, go to
https://www.nature.com/articles/s41467-018-03548-7
https://www.llnl.gov/news/experiments-shed-new-light-supernovae

Harper excels at defense; reflects on time at SC

Doctoral student experience

My experience as a computational science graduate student definitely bore the hallmarks of engineering. I find that the mentality in approaching the work, the expectations, and the hours I ended up being physically present in the laboratory were much more rigorous because of the desire I had to try to meet the expectations of the engineers. It was a great experience though.

During my first weeks there, I was needed to help complete and troubleshoot the source-code from another researcher who suddenly became unavailable. There was to be an assessment from our funding agency in two weeks and without this software completed, the robot would not be able to function. I had very little experience in the lab at this time, but I sat and rebuilt much of the code that I could understand, taking almost every waking hour during these two



weeks. The day before the assessment, we were able to get the robot operational. It may not seem like much now, but at the time it was a herculean effort. Through all of this, the entire team of researchers at the lab was there early every morning and late into the evenings, even though much of the software work hinged on me, no one abandoned the new guy and every person gave it their all. Engineering work is not always easy or fun, but it is also never done alone, I learned a lot about good teamwork in these few days. In the end, the robot was successful in running tests and we were approved for another few years of funding.

On another occasion, I was happily working (I had a team at this point) on a project that I was interested and comfortable in. The director of the lab stepped into the room and saw me, smiled, and asked me if I was interested in taking on an interesting project. I was working on two papers at the time, but he had never steered me wrong before so I said, "sure thing, what is the project?" A frenzied three weeks of activity culminated in the very first motion planning capable dynamic climbing robot. I worked very closely with other students who were experts in locomotion, controls and dynamics and added my abilities in AI and motion planning. It was humbling to work closely with people who are amazing with what they do, we are still good friends now. Together we made a significant contribution to the field of robotics. I could have never done it by myself.

About CISCOR [Center for Intelligent Systems, Control & Robotics]

My entry into the CISCOR lab was certainly an interesting adventure. I started my first semester here at FSU in the Department of Scientific Computing, and was happily completing the required courses. I was a little worried about summer funding (I was a TA for PIC when I started.) and had arranged to work with Xiuwen Liu in the CS department. One day while working on a proposal with Xiuwen, I had a feeling that I should check for a robotics lab and see if they could use me. It was a strong enough feeling that I dropped everything and applied that day.

It turned out that the CISCOR lab was about to advertise for a new computer scientist student to work in algorithm development. My application came in on the day they were planning to post it; in fact, the director called me only a few moments after my application was submitted because of this. I was able to explain my background and he was incredibly happy to find a person who had a mathematics and physics background coupled with computer science. I was brought on as a volunteer to see what I could do, but in short order, I was working on a series of projects for the lab.

What's next

I am leaving CISCOR to move on to my next great adventure but the memories there are wonderful. I paid for all of my accomplishments in painstaking work, but I was surrounded by what I consider to be some of the greatest minds and people in the world. This is important to me; in fact, I turned down a post-doc offer from MIT's Computer

Science and Artificial Intelligence Lab (CSAIL) partly because I knew that the people would be harder to get along with. The job which I did end up accepting also has amazing people who are willing to stand up and choose to be good.

On coming to FSU

As it turns out, I was not planning to go to FSU; it wasn't until someone mentioned that FSU has a scientific computing department that I even knew about the field. When I looked that evening at the program, I noticed that the application window had closed, and on a whim, I sent an email to Dr. Peterson asking if they were still accepting applications. She told me to send my information along and if they thought I was a good fit, they could consider me as the applicant process had only just started.
What was surprising was that FSU was the last school that I had applied to but one of the first ones to respond. All of the dialogue that I had with people was pleasant and the freedom in taking courses sounded very nice. I ended up turning down a CS program at Purdue, Minnesota and the scientific computing program at George Mason to come to FSU. It was a great decision.

As a Ph.D. student, I have had an incredible opportunity for growth here. I began with little capacity to write, but have since published thirteen papers (some of which are currently under review) and many technical reports. I was not super comfortable standing in front of a room full of intelligent people and presenting, but have learned to enjoy presenting my work to my peers. I have accepted invitations to give talks at my alma mater (University of Utah), BYU, MIT, and JPL along with several companies that were interested in my work. Every day was treated as a great day for growth. Each day was not always full of technical research but it was always full of learning.

In fact, there were some days when I did not have the chance to even turn on my computer. One meeting followed another and people needed something here or there and the day would just disappear. There was a time it was so bad that the director actually sent out an email telling people to let me work. Those were fun days too; I learned a lot about time management, prioritization and goal setting as well as what it means to mentor and manage a team.

Advice to new researchers

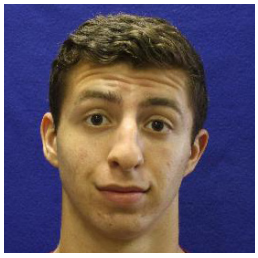
Don't get stuck in analysis paralysis, there are always more papers to read. Whatever you know now, whatever technical ability you can apply now is sufficient to get started. Just try something -- that will give you wisdom to keep pressing forward.

Mario Harper is a senior data scientist at Progressive Leasing. For more, go to sc.fsu.edu.

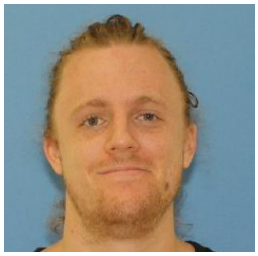
Harper's Projects

- Advanced Optimal Resource Allocation (AORA): How does a micro-grid power system allocate resources to maximize profits and mitigate wear and degradation of individual components? A team that I was a part of designed this algorithm and tested it with hardware-in-the-loop tests at the Center for Advanced Power Systems (CAPS).
- Load Control in Large-Scale Power Systems: Can AORA handle complex power loads? Does the optimizer have the ability to control the variable load intelligently? It turns out that it can! This product is actually now under patent rights and we got a good proposal funded for a STTR because of it.
- Walking Improvement for Parkinson's Patients: Can our understanding of gait dynamics and body stability help new treatment and therapy procedures for patients in advanced Parkinson's? In this project headed by the FSU medical school, I was able to help deliver the data collection and measurement software that was needed to quantify how the patients were actually performing. It turns out that we were able to measure performance improvement and some patients said, "they had not walked like this in years."
- Technical Integration Lead (RCTA): I headed the large project in the Robotics Collaborative Technology Alliance (RCTA) on our capability group. I had the opportunity to network with researchers from JPL, MIT, CMU and other leading robotics institutions as my responsibilities included ensuring that the RCTA robotic assets were functioning with all developed technologies by those and our groups.
- Terrain Aware Motion Planning: Just what it sounds like. Can we be aware of our terrain as we plan the optimal trajectory for our robots to move? Yes, yes we can. Vegetation that is traversable, mixed terrains and non-traversable regions were effectively considered and modelled by our algorithm.
- Legged Robots: High speed motion using legs is hard for young humans to do right. (I know, I have kids.) This is particularly true for dynamic legged robots. Much of my core contributions to the field of robotics is in the algorithmic development of motion planners that now make it possible for these robots to navigate while honoring their natural dynamics.
- Climbing Robots: We are the very first institution to implement a motion planner for a dynamic climbing robot. No one else in the world has the technology needed to do complex planning like this, go team! This was one of my favorite algorithms I got to develop.
- Multi-Modal Planning Paradigm: Can a planning algorithm handle energy based planning, time efficient planning and distance optimal planning? Yes, yes it can... at least it can now.
- Mentoring: My favorite projects. It can scarcely be called a project, but I took great joy in having many people come into my sphere of work. Many students interested in robotics as well as new undergraduate students looking to take a stab at research came by my desk and I found a myriad of interesting projects to work on with them. One of my favorite memories is my now good friend coming up to me and saying, "I had an exam on coding and after working a few months with you, it was the easiest thing ever. I aced it." I have had quite a few students; it has been a wonderful experience.

New grad students, new staff at DSC



Austin Eovito



Cody Ficarra

Albert (A.J.) Iglesias

Scientific Computing graduate student Austin Eovito claims many places as home. As the son of a United States Marine Corps officer, he and his family moved frequently - every two years - for most of his life. Eovito's favorite location was Okinawa, Japan, where he lived for almost four years, the longest he lived anywhere.

After finishing high school in Jacksonville, Florida, Eovito pursued his undergraduate degree in Applied Economics at FSU. During his senior year, he worked as Data and Analytics Manager at the DeVoe L. Moore Center, an applied public policy research and teaching center on campus. There, Eovito studied the Tallahassee Redevelopment Agency and white-collar crime. His current research with Gordon Erlebacher uses natural language processing.

When he is not doing research or school work, Eovito enjoys spending time with his fiancé Marissa, his dog Balto, and cat, Max. He also enjoys reading [his interests tend toward philosophy, history and leadership], archery, and drone videography.

A Florida resident through and through, new grad student Cody Ficarra was born in Fort Walton Beach and grew up in nearby Santa Rosa Beach, just a few hours west of Tallahassee. Ficarra received his Associate of Arts degree from Pensacola Community College, then transferred to FSU to complete a bachelor of science in psychology with a minor in scientific computing.

As an undergrad, Ficarra worked with psychology and neuroscience professor Richard Hyson to research neurotransmitters involved in the neuronal path of African finches. One of his current projects involves coding a numerical model for the calcium dynamics of an astrocyte with Ph.D. student Evan Cresswell.

When he has free time, Ficarra enjoys spending time with Carly, his girlfriend of four years and playing video games. He also enjoys outdoor activities, working out, and playing video games.

Albert (AJ) Iglesias comes to Scientific Computing from Miami, Florida after obtaining his undergraduate degree at FSU that shows his many intellectual interests. Iglesias completed his Bachelor of Science degree in biology with three minors – chemistry, interdisciplinary sciences, and psychology. He is now a masters student in computational science.

While an undergrad, Iglesias studied human sciences and nutrition with FSU Professor of Nutrition Food & Exercise Science, Bahram Arjmandi. Their research focused on the effect of dried plums on bone health, and the effect of certain bean diets on hamsters without ovaries. Following completion of the program, he plans to work in software development and artificial intelligence.

In his leisure time, Iglesias chooses from a host of activities. He enjoys working out at the gym and going to the beach, and watching and playing sports [football, soccer and basketball]. He also enjoys traveling.

Young Hwan Kim calls South Korea home, but feels a special link to China, as he spent much time there during his childhood due to his parents' work. Kim studied biochemistry and computational math at Asbury University, a small school in western central Kentucky, graduating in 2018. While a student at Asbury, Kim did a research internship at the University of Kentucky that led him to study the devel-

opment of an efficient nicotine-metabolizing enzyme. He has not yet settled on an advisor, but is interested in continuing his biomedical research.

In his leisure time, Kim enjoys talking with people and relaxing with his wife. He enjoys playing board games, watching Netflix, playing chess and trying new foods.

A new SC masters degree student, Jonathon Nosowitz hails from Long Island, New York, having completed his undergraduate degree in computer science with a double minor in math and physics at Iona College in New Rochelle. While at Iona, Nosowitz was active in campus activities: he was a drummer for the band, a member of national and international honor societies, and was involved in research and conference presentations.

Nosowitz was a participant in NASA's Undergraduate Research Associates in Astrobiology program in 2016. He analyzed high-resolution infrared Mars spectra, leading to a comprehensive infrared spectral survey and to a sensitive search for organics, new bands of carbon dioxide and water. The new survey revealed several unknown spectral features that could be related to new molecular bands. Nosowitz is working with Tomasz Plewa on his investigations of supernovae.

In his free time, Nosowitz enjoys playing tennis, traveling, and seeing historic sites; he has traveled domestically and abroad.

Kevin Ziegler was born in Bowling Green, Kentucky, then attended the University of Alabama after high school, earning dual degrees in biology and computer science in May 2018. As an undergrad, Ziegler studied the detection and prevalence of Chytrid fungus in bullfrogs in Warren County Kentucky. During a summer internship, he did research on the effect of changing the grid resolution of the Weather and Research Forecasting climate model.

Since June, Ziegler has worked with Alan Lemmon on two projects. The first project studies whole genome sequences for a group of organisms in an effort to generate distributions for different kinds of organisms (Vertebrates, Primates, Flies, Humans, etc.). The goal is to see what location and region of the genome should be taken to create an accurate and resolved gene tree for the species they are working on.

The second project involves adding a sophisticated analysis to Phylomapper, Lemmon's software program. Phylomapper uses a maximum likelihood Bayesian framework to approximate ancestral locations of a population given the gene tree of that population. The program is based on the relationship between physical distance and genetic distance; it tries to come up with the most likely physical separation that explains the genetic separation. Ziegler and Lemmon are working on a resistance raster based on variables such as elevation, temperature, and water. The resistance raster would provide information on the obstacles a population encountered in a particular location.

In his free time, Ziegler plays ultimate Frisbee among other outdoor pursuits such as hiking, where he goes for animal spotting. He is looking forward to getting out to the Apalachicola National Forest in the near future.

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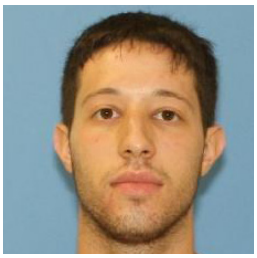
see New, p8.

Young Hwan Kim



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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.

New, continued from p. 7

Lisa Montgomery

Tarlisha (Lisa) Montgomery is the department's new Administrative Associate. In her new position, Montgomery is the travel representative for the department. A Tallahassee native, she comes to Scientific Computing from the Department of Health. Prior to that, she worked at the Departments of Juvenile Justice, Revenue and Education. She is also a veteran, having served in the U. S. Army at Fort Jackson, South Carolina.

In her new role, Montgomery assists faculty, students and staff in making travel arrangements and getting reimbursements, initiates requisitions for purchases, communicates with vendors to facilitate acquisitions, prepares appointment papers, monitors time and leave, and is responsible for payroll corrections, certifications and other human resource reporting.

Montgomery is a graduate of Godby High School and Tallahassee Community College; she has a deep and abiding interest in guiding young adults through mentorship, and plans to continue her education in social work. She is the proud parent of two children. Her daughter Courtnei is a senior at Florida A&M University; her son Corey is an 8th grader at Fairview Middle School. When she has time, Montgomery likes to cook and read.

Michelle Claycomb was recently promoted to Administrative Specialist. Claycomb has been with the department since May 2017, and applied for the position because she was interested in new responsibilities and new challenges.

Since accepting the position, Claycomb has become in tune with a larger picture of the department's operations and goals, and how to make the most of the department's resources.

For more, go to sc.fsu.edu.

sc.fsu.edu