Summer 2020

Department of Scientific Computing

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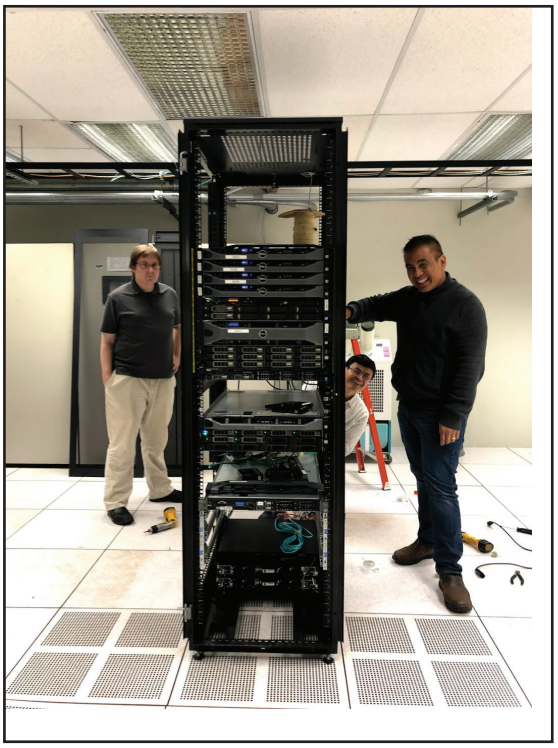
Technology staff transitions department on line

The DSC Technical Support Group (TSG) has always played a vital role in the department, providing services to computationally sophisticated scientists and staff with high end user needs. Before COVID-19, the department was a leading adopter of education technology; for years, the Seminar Room and Visualization Laboratories have been home to sophisticated, high quality equipment for the department and other university users. Since the pandemic, however, the unplanned and rapid shift to online administration and web-based learning and research has caused a significant surge in technology usage.

With the help of TSG staff – Bill Burgess, Amado Cruz, Xiaoguang Li, Michael McDonald and John Thompson – and technology, the department has continued to thrive.

"Staff members together with students, Jake Cherry and Young Hwan Kim, are working on a number of projects and discussing progress regularly," said Xiaoguang Li, TSG Systems Administrator. "The group has addressed the power outage to several core system devices due to the monthly power generator test. With the help of Ashley Gannon, a cooling system draining issue is also rectified."

TSG has been able to smoothly anticipate and implement everything the department needs, from training administrative staff on how to use the university's Virtual Private Network to using a previously rarely used software for a successful virtual Computational Exposition, to issuing new laptops for working off-site and troubleshooting on the fly.



Technical Support Group members, John Thompson, Xiaoguang Li, & Amado Cruz enhance DSC network switching infrastructure. Photo courtesy Michael McDonald.

"We are doing more screen sharing and remote troubleshooting than anytime in the past," Li observed.

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SC faculty awarded grant to study filtration processes

SC Assistant Professor Bryan Quaife

A $250,000 grant has been awarded to Scientific Computing Assistant Professor Bryan Quaife toward his research on understanding and modeling naturally occurring porous and granular materials in groundwater flow. The National Science Foundation (NSF) provided the funds as part of its Computational Mathematics section of the Division of Mathematical Sciences. The Computational Mathematics section supports mathematical research in areas of science where computation plays a central and essential role, emphasizing analysis, development and implementation of numerical methods and algorithms, and symbolic methods. The ultimate aim of the grant is to develop a suite of computational tools geared towards developing a deeper understanding of the physical processes by which groundwater flow alters porous-media properties and to characterize the changes that occur as the medium evolves over time.

"Groundwater flow occurs in complex networks, such as karsts, that formed over long periods of time by processes such as erosion and dissolution," said Quaife. "Understanding the formation of these geometries is critical to describe transport properties in these geometries and to predict catastrophic effects such as sinkholes."

The grant research will continue for the next three years, and will support a doctoral student for whom the work will serve as the foundation for the dissertation.

The research will help us understand how naturally occurring porous and granular materials, such as soil, sand, and clay, play a pivotal role in regulating earth's water resources by filtering contaminants and, over long timescales, supplying fresh water.

Not only is this process essential for human water resources, but also for the ecology of rivers, estuaries, and other natural habitats. These natural water resources have been placed under enormous pressure by human population growth and associated activities that can compromise the natural filtration cycle, such as expansion of industry, urbanization, pollution, and climate change.
An important benefit of the proposed research is the immersion of a graduate student in cross-disciplinary research. This proposal involves a confluence of disciplines, most centrally computational mathematics, but also geophysics, environmental science, hydrology, and physical modeling. Exposure to a range of disciplines is, in the view of the PIs, an invaluable opportunity for young scientists.

In addition to the research, the project places a particular focus on community outreach and involvement to all – the public at large, graduate students, undergraduate students and students in kindergarten through 12th grade.

"FSU's connections with the community will be utilized to engage others in the research. Aspects of the research are accessible to young scientists that will be secured through

> "[T]he research will be showcased to the local community, and particularly school-aged children, through events such as FSU's Math Fun Day and the Tallahassee Science Festival."
> ----------Bryan Quaife

programs such as the Undergraduate Research Opportunity Program (UROP) and the Young Scholars Program (YSP)," Quaife commented. "In addition, the research will be showcased to the local community, and particularly school-aged children, through events such as FSU's Math Fun Day and the Tallahassee Science Festival."

The grant was secured through a collaboration between Quaife and Nick Moore; the two will work in concert on the project. Moore is a mathematician and scholar whose expertise includes modeling dynamic interactions between fluids and structures, especially geophysical and biologically motivated settings.

This grant is Quaife's first award from NSF. Since joining the Scientific Computing faculty, Quaife has contributed to the department with his research, grant awards, and mentorship. He has received grants for projects in excess of $2.5M, published prolifically, presented research findings throughout North America, and mentored a host of masters and doctoral students.

Quaife holds a doctorate in applied and computational mathematics from Simon Fraser University in British Columbia, Canada, a Master of Science in applied mathematics from the University of Calgary (UCalgary) in Alberta, and a Bachelor of Science in pure and applied mathematics from UCalgary.

For more on Quaife, go to http://people.sc.fsu.edu/~bquaife/.

For more on the Department of Scientific Computing, go to sc.fsu.edu.

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Teaching and administrative services, too, continue uninterrupted; technology is playing a vital role to make life, communication, working from home, and getting services and products relatively easy. Faculty and staff use Canvas for online classes and Zoom, a cloud-based video conferencing service, for virtual meetings, discussions and reporting. The department's academic advisor, Karey Fowler, reserves blocks of time for student recruitment, course registration and advising consultations.

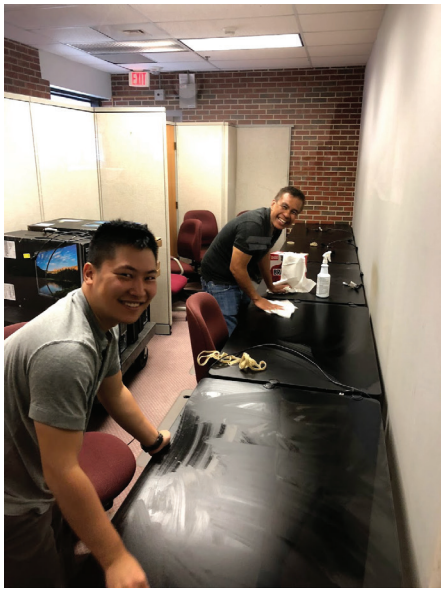
TSG's efforts have been felt by everyone in the department. "We have discovered in these last few months that many previous face-to-face interactions proceed smoothly online with some new advantages," said DSC Chair, Gordon Erlebacher. "People are more readily available, it is possible for multiple participants to share information, we can organize ad-hoc meetings, colloquia and workshops with colleagues around the world, and attend workshops and conferences at much lower cost. Some of these new operational procedures will surely persist once life returns to normal."

Even with social distancing and remote work, purchase orders continue to go out, with a new procedure for confirmation and delivery of goods; administrative staff have implemented the coordination required to facilitate faculty promotion and tenure, and the department has become facile with big and small tech to continue smooth operations while staying safe.

Erlebacher remarked, "We are proud of how our administrative and technical staff have managed this crisis, rising to the occasion, and sporting a positive and flexible attitude. Thank you!"

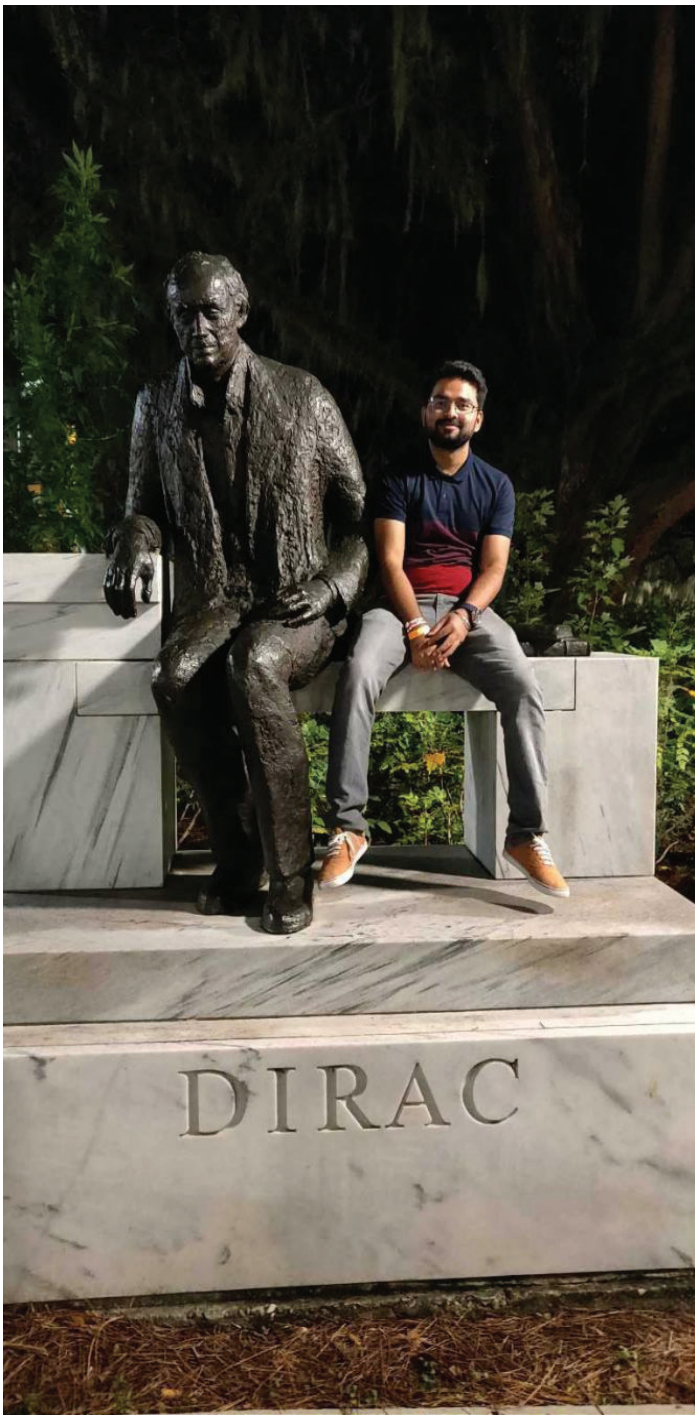
"With the continued dedication of staff members as well as student workers, social distancing will have little impact on meeting the needs of our department," said Li.

For more on TSG and the department, go to sc.fsu.edu.



Right: Technical Support Group members Young Hwan Kim & Amado Cruz, sanitize the hallway computer lab. Photo courtesy Michael McDonald.

Doctoral student accepts internship at national lab



Pankaj Chouhan sitting at the Paul Dirac statue adjacent to the Dirac Science Library at Florida State University.

Ph.D. student Pankaj Chouhan scored an internship for the summer, working at Argonne National Laboratory. He talks about his search for the position, and what it's like to intern remotely.

When I joined the department, I talked with different graduate students about their work and what they thought about the department and the opportunities being here offers. While talking with Brian Bartoldson, he mentioned that he did a couple of summer internships at Lawrence Livermore National Lab. He said that it's a good opportunity not just in terms of career building. He said he also gained a lot of experience and he used the opportunity to make good connections in a short amount of time. I really liked the idea, especially when I learned more about national labs from Ezra Brooker who had an internship at Los Alamos. Ezra talked about some of the good research people from our department have been doing; that was when I made up my mind to try to get an internship at a national lab too. After all I had heard, I thought doing so would be a good career strategy.

I wanted to apply in the fall - September and October - since that is the ideal time to start, but as I was in the middle of the semester, and had other responsibilities, I wasn't able to find the required time to work on the applications. So I decided to give it a chance during the winter break. I went to all national lab sites and copied down the project in the computational domain that I liked most, what they are asking for - statement of purpose, resume, etc. - and I also made sure about the due dates, and other sorts of formalities. It took me around 6-8 days to prepare all the materials for my applications, and I applied to 4-5 national labs. Since most of the labs follow similar application procedures, after getting materials ready for first application, it's quite easy to apply to other labs.

I will be working on a project supervised by Dr. Olle Heinonen. He is a condensed matter theorist and computational materials scientist in the Materials Science Division. Recently, he became interested in artificial intelligence (AI) applications in materials sciences. One research project he leads focuses on developing and applying quantum Monte Carlo (QMC) methods in materials sciences. Because QMC is a statistical method, it is noisy (has unexplained variation or randomness), and it is very expensive to reduce the noise. So my job is to come with an AI framework using neural networks to denoise the images generated using QMC. This project is interdisciplinary; aside from Dr. Olle I will also be collaborating with Dr. Sandeep Madiredy, a machine learning expert, and Dr. Hyeondeok Shin, a Monte Carlo expert in computational science, both at Argonne.

I hope to learn as much as I can about computer vision during this internship. I believe this is one of the fields which will remain significant in the future. If possible, I will try to make a substantial research contribution so I can be a part of any publication coming out of this work. When I found out I would work virtually, I was quite disappointed. One of the most important aspects of an internship is making connections with all sorts of people from different fields, and an online internship won't have that element. I am quite lucky that my research supervisor at DSC, Dr. Sachin Shanbhag and my supervisor at Argonne, Dr. Olle, both make time for me whenever I feel like I need to have a discussion. Although I was very excited with the prospect of moving to Chicago, I believe that I will be able to do the same quality work that I would do in normal circumstances.

"I hope to learn as much as I can about computer vision during this internship. I believe this is one of the fields which will remain significant in the future. ..... I will try to make a substantial research contribution...."

----- Pankaj Chouhan

For more on Chouhan's research with Dr. Heinonen, go to anl.gov.

Below: Aerial photograph of Argonne National Laboratory, a Department of Energy multidisciplinary science and engineering research center located in Illinois by the University of Chicago.

Summer brings new graduates

DSC MS grad Daryn Sagel

Daryn Sagel, a fire dynamics student, has completed the requirements for the Master of Computational Science degree. Sagel was co-mentored by Bryan Quaife and Kevin Speer.

During her year as a student, Sagel was active in the department's research and outreach projects, having facilitated the Geophysical Fluid Dynamics Institute's involvement in Create with Code!, a summer camp for local high school students to introduce Python for data visualization, machine learning, robotics programming, and game design. Sagel's thesis, A New Way to Look at Fire: Computer Vision Applied to Fire Dynamics, presents a new approach for examining fire spread. Application of adapted computer vision principles to visual and infrared video allowed Sagel to capture fire, wind, and plume behavior without specialized instrumentation. Her research helps quantify the transport of heat and fire spread, turbulent statistical information, and plume structure through modifications of classical computer vision algorithms with adapted graph theory techniques. This work can be applied to diverse instances of the environment and used to extract data from prescribed fire videos. These data extraction experiments improve our understanding of the dynamics in complex environments and can validate fire spread models.

Sagel is currently working with VayuAI in wind physics, data science, cloud computing, and machine learning while continuing fire dynamics research and working on publications.

In his dissertation research, Brian Bartoldson studied how pruning (removing) neural network parameters affects the network's ability to accurately classify previously unseen inputs (generalization performance). While pruning is known to help generalization, the reason for this was unclear. Bartoldson's studies found support for a novel explanation of how pruning helps.

Neural networks are machine learning algorithms that learn to perform a task using example data. The goal of pruning is to remove some of the network's parameters during the learning process to improve efficiency and generalization. Pruning deep neural networks makes them smaller and faster, and thus more useful in applications requiring low resource usage (mobile devices) or fast response times (self-driving cars). Despite their sometimes massive size, neural networks are popular because of their

Brian Bartoldson, Ph.D.

ability to generalize well, which a large part of the machine learning research community is focused on trying to explain.

By shedding light on how pruning helps the generalization of neural networks, Bartoldson sought to address a piece of the generalization puzzle in *The Generalization-Stability Tradeoff in Neural Network Pruning*, a paper coauthored by fellow researchers Ari Morcos, Adrian Barbu, and Gordon Erlebacher that previews more extensive work done in Bartoldson's dissertation.

In the fall, Bartoldson will continue studying machine learning and neural networks as a Machine Learning Postdoctoral Research Staff Member at Lawrence Livermore National Laboratory.

Recently, Eitan Lees defended his dissertation on the study of corrosion in metals. Corrosion adversely affects the performance of metal alloys that are widely used as structural materials in the automobile, naval, and aircraft industries. Lees' work presents a simplified multiphase (solid, liquid, and porous interphase) nonlocal model for pitting corrosion in aluminum alloys.

He proposes and solves nonlocal reaction diffusion equations and applies the nonlocal model to the one dimensional liquid junction problem in which two electrolyte solutions are transported through a permeable membrane. The title of his dissertation is *A Simplified Nonlocal Model for Local Corrosion*.

While completing his doctoral work, Lees taught the introduction to scientific computing course for new students joining the department and became involved with the open source community, contributing mostly to a Python visualization library named Altair

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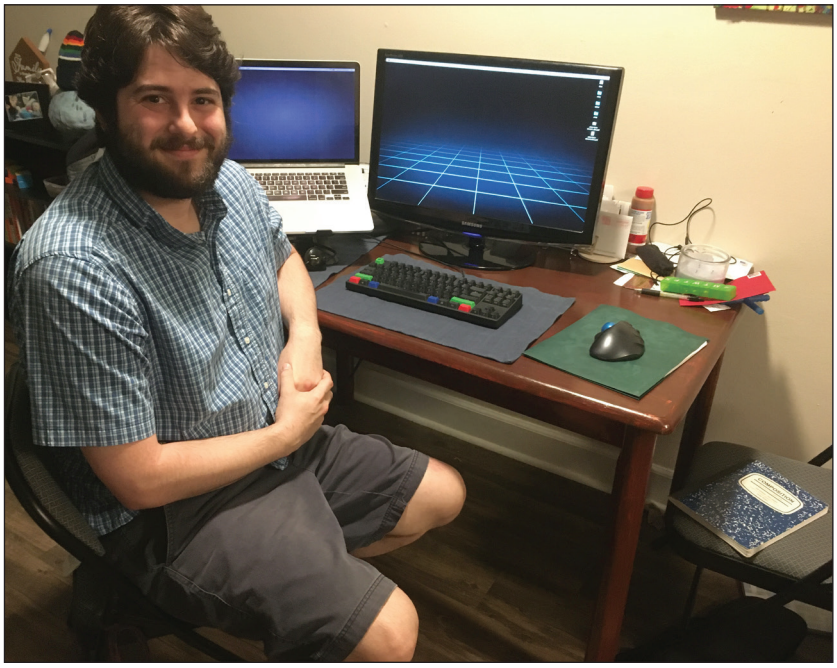
For more on Bartoldson, Lees and Sagel, go to:
https://www.sc.fsu.edu/



Right: Recent doctoral grad Eitan Lees

Department of Scientific Computing
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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.

Coming up....

Brandon Gusto wins SMART Scholar award

Kevin Speer joins Scientific Computing

DSC Senior interns at NASA

These stories and more in our next edition. Stay tuned!

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