MESSAGE FROM THE DIRECTOR

Welcome to the inaugural SimCenter Annual Report for Fiscal Year 2018 (July 1, 2017–June 30, 2018). As Director of the SimCenter, I am proud to share selected examples of excellent research and activities of several of our professors, students, and alums.

SimCenter, the Center of Excellence in Applied Computational Science and Engineering, is UTC’s Research Accelerator and Research Computing Core Facility. SimCenter is a THEC-funded research organization designed to advance modeling- and simulation-based science at UTC. Founded in 2002 as the home of the Computational Engineering Ph.D., SimCenter was re-inaugurated in 2017 with a broader, campus-wide mission that builds on its original mission to enable modeling and simulation, high-performance computing, data science, machine learning, and growth in UTC’s Ph.D.s programs. Further, SimCenter supports faculty with competitive proposal development, funding, and grants management, including temporary research space where applicable.

Here, you will see the breadth and depth of faculty and student research, development, and outreach enabled by SimCenter seed funding and research computing infrastructure. Contributions from faculty in Mathematics, Computer Science and Engineering, Electrical Engineering, Mechanical Engineering, and Chemical Engineering are represented here. The work presented here keys to our “swimlanes” or emphasis areas.

During FY2018, active swimlanes included Aerospace & Defense, Cybersecurity & Cyber-physical Systems, Energy & the Environment, Health and Biosystems, High-Performance Computer Systems/Algorithms, and Smart Cities. The Smart Cities swim lane, helmed by Dr. Mina Sartipi, graduated at the end of the fiscal year into its own UTC center named CUIP, Center for Urban Informatics and Progress. SimCenter seed funding and support to Dr. Sartipi and her colleagues has helped UTC launch this exciting, interdisciplinary academic center.

SimCenter’s goal is also to make contributions and positive impacts beyond UTC and engage new participants from the community, state, and region. We look forward to an ever-expanding portfolio of R&D centered on modeling and simulation, high-performance computing, and advanced algorithms in our swimlane areas and beyond.

Sincerely,

DR. ANTHONY (TONY) SKJELLUM has been the Director of the SimCenter since August 2017. He received his B.S. in Physics and his M.S. and Ph.D. in Chemical Engineering from California Institute of Technology in 1984, 1985, and 1990, respectively. He led the R&D in HPC and cyber at Auburn University in the College of Engineering for just over three years prior to joining UTC as a Professor of Computer Science, Chair of Excellence, and the new SimCenter Director. Dr. Skjellum’s research interests are, generally, in parallel computing and MPI. His current research group is a split between cyber/Internet of Things and HPC and Exascale Storage, and he holds active grants from DOE/NNSA and NSF.

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The SimCenter is a research center for multidisciplinary research at UTC. It not only serves as a research incubator for innovative concepts and laboratories but also acts as UTC’s core facility for High-Performance Computing and Storage.

UTC has two new concentrations in Computational Science: Computer Science and Computational Math. These concentrations are in addition to UTC’s initial Ph.D. in Computational Science: Computational Engineering. All of our Ph.D. and some of our M.S. and undergraduate students are now housed in the SimCenter. The facility includes faculty offices; student cubicles; a 1,500-square-foot computer room; a conference/meeting room that accommodates 25 people; an 80-seat auditorium; and two secure expandable suites of rooms dedicated to proprietary and/or classified research, a research library, and other work space. The interior layout is designed to facilitate extensive interdisciplinary interactions among faculty and students, with student cubicles in large open spaces adjacent to faculty offices. Researchers also have access to the high-performance clusters.

In FY2018, we added the following pieces of crucial computing equipment to the SimCenter’s available resources.

**VMWARE Infrastructure**
This system is mainly used to run services in a virtual environment, e.g., authentication, print servers, helpdesk, wiki, and several research-related virtual machines (VMs). We will be migrating these research VMs into another Research as a Service (RaaS) environment early next year; then, this VMWARE setup will support only infrastructure and services. The system is a redundant, highly available, three-server system with over 20TB of local storage.

**DDN Storage**
This addition is a significant one for the SimCenter, as it provides an extra 1.1 PB of storage capacity. It runs IBM’s Spectrum Scale parallel filesystem software and provides our users with their home directories and research/“scratch” space. This system has two tiers: a tier of fast storage (~100TB) for home directories (all backed up) and a capacity tier (~1PB) for the “scratch” space.

**IBM Power9 (lookout) Cluster**
This cluster consists of four IBM Power9 AC922 servers with four socket-based NVIDIA Volta GPUs in them. These machines are fine-tuned for HPC/AI and are quite powerful. They are almost identical to the ones that currently comprise the fastest supercomputer in the world today at ORNL, the only difference being that ours only have four GPUs in them (compared to six).

**New Tape Backup**
One minor but important addition to our resources is a new tape backup system that backs up our new storage as well as the VM infrastructure/systems in the VMWARE system.

**New Fire Suppression System**
Another less exciting but equally important change is our shift from a water-based fire suppression system to an inert gas one, which ensures our servers will never get wet!
The UTC Center of Excellence in Applied Computational Science and Engineering (CEACSE), or SimCenter, continues its second decade of invigorating scientific inquiry, bolstering the learning environment, broadening participation, and establishing sustainable research pathways that benefit our institution, faculty and students, and the State of Tennessee. FY2018 marked CEACSE’s thirteenth year of growing UTC’s first Center of Excellence into a critically important incubator for inquiry and experimentation across a diverse array of computational science and engineering endeavors. CEACSE comprises the indispensable factor that enables UTC to recruit, retain, and engage outstanding professors and equally outstanding students through research experiences for undergraduates up to and including Ph.D. students.

CEACSE research and advanced development activities enhance education at all academic levels at UTC including through the Ph.D. program in Computational Science. Graduate and undergraduate students alike participate in various research activities and experiential learning as a result of current and prior CEACSE funding. Companies in our community and region continue to grow their interest in the educational programs impacted by CEACSE initiatives, in large measure because of the applied R&D supported by CEACSE. SimCenter, the central site of CEACSE, continues to broaden and deepen efforts to partner with companies in the Chattanooga region and beyond. Because of increasing capabilities in high-performance computing and the overarching importance of modeling, simulation, and advanced computing in research and education, the efforts and outcomes of our researchers and their students will continue to serve as research anchors that attract students from across the nation and internationally. These students represent a valuable contribution to the future workforce of knowledge workers for the community and the state of Tennessee. Company leaders tell us time and again how important the core competencies of our Center of Excellence are and how valuable our graduates are to their business enterprises, including local high-tech startups.

**Notable Outcomes of FY2018**

The Smart Cities & Urban Dynamics swimlane graduated into its own research center at UTC: Center for Urban Informatics and Progress (CUIP). This center’s inaugural director is Dr. Mina Sartipi, who led the original swimlane and continues to lead campus-wide efforts on Smart Cities and related R&D. Support from CEACSE leveraged into external support from NSF and others and has now enabled this second academic center to emerge on campus. SimCenter will continue to be a resource to CUIP, and faculty associated with it continue to submit proposals in the modeling and simulation area related to smart cities.

Dr. Don Reising has assumed the leadership role for the Energy & Environment swimlane. Dr. Craig Tanis has assumed the leadership role for the new swimlane for HPC and Algorithms. Dr. Farah Kandah has assumed the leadership role for the swimlane for Cybersecurity & Cyber-physical Systems. We have established research focus groups for Health & Biological Systems as part of the swimlane now led by Dr. Hope Klug, who is now also the Interim Chair of Biology. Two interdisciplinary research tracks are active as of November 2018: Hospital Health Modeling & Simulation and Interdisciplinary Math/Computer Science/Biology & Ecology Ideation.

Additionally, Dr. Eleni Panagiotou was hired as a new professor of mathematics. Her work in modeling and simulation applies to problems with complex physics and geometry in biological and chemical engineering (e.g., rheology) and many other application areas.

**Important Technical Advancements in FY2018**

Dr. Robert Webster was funded by Engility Corporation for “Heterogeneous HPC for High-order Stabilized Finite-elements on Moving and Deforming Domains”; Dr. Abdollah Arabshahi has implemented and validated the third-order MUSCL-type numerical flux formulation scheme and extended to higher-order accurate (up to ninth-order spatial accuracy and second-order temporal accuracy) weighted essentially nonoscillatory (WENO) scheme in the structured flow solver for high-speed flow simulations; and Dr. Tony Skjellum received R&D support from NSF in HPC for the project entitled “Next-Generation Message Passing for Parallel Programming: Resiliency, Time-to-Solution, Performance-Portability, Scalability, and QoS.”

Dr. Hong Qin (Computer Science, PI) together with Drs. Hope Klug (Biology), Joey Shaw (Biology), Jennifer Boyd (Biology), and Azad Hossain (Environmental Sciences) received a major National Science Foundation (NSF) Award for Big Data R&D entitled “Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education Award.” This work will be supported by SimCenter as it kicks off in October 2018. Our goal will be to connect Big Data outside UTC with SimCenter infrastructure that will support these faculty members and our Health & Biosystems and Energy & Environment swim lanes. All of the professors involved have received current or prior CEACSE funding support.
Dr. Skjellum’s research group, together with collaborators at Clemson University, launched a new blockchain technology based on funding from NSF, keyed to data provenance. This work has direct impact on HPC workflows, and the team has expanded its scope and incorporated collaborators at the University of South Carolina and the University of Alabama at Birmingham to explore HPC Workflows, reproducibility, and data provenance. Collaborations in this area and in blockchain have commenced with Oak Ridge National Laboratory (ORNL) as a consequence of this R&D work.

The SimCenter research network infrastructure was updated to support Internet of Things, smart cities prototyping, and cyber/systems activities. This specialized network allows scientists and engineers to work in parallel with the university’s production network while avoiding security concerns. This update is a prelude to supporting a DMZ, data transfer node, and other research infrastructure in FY2019 and beyond. SimCenter received an IBM Award for Machine Learning R&D ($20,000) and regional collaboration in federated clouds.

In collaboration, College of Engineering and Computer Science (CECS), SimCenter, and the Office of the Vice Chancellor for Research foster a rapidly expanding and enhancing culture of securing external funding as an outcome of seed research funding provided by CEACSE. We recognize the challenges for faculty to excel in attracting extramural funding while meeting all aspects of meritorious scholarship. We provide support through the Office of Research and Sponsored Programs (ORSP), through focus on opportunities that are designed to lead to larger funding awards, and through development of strategic partnerships. CEACSE is emerging as the nexus of UTC research incubation and acceleration, HPC and data science, and is a key provider of faculty resources that complement and supplement ORSP’s offerings and add to those of faculty home departments. We are also UTC’s Research Computing Core Facility, supporting the growing demand for High Performance Computing in Modeling, Simulation, Data Analytics, and Machine Learning.
DR. MINA SARTIPI is the Founding Director of the Center for Urban Informatics and Progress (CUIP) and a UC Foundation Professor in the Computer Science and Engineering Department (CSE), where she leads the Smart Communications and Analysis Lab (SCAL). She received her B.S. in Electrical Engineering from Sharif University of Technology, Tehran, Iran, in 2001, and her M.S. and Ph.D. degrees in Electrical and Computer Engineering from Georgia Tech in 2003 and 2006, respectively. Dr. Sartipi’s research interests are in communications and data science—in particular, advanced wireless communications and data analysis for smart healthcare and urban futures. She has served as the technical program chair of numerous conferences in wireless communications and networking.

In 2008, Dr. Sartipi was named UC Foundation Assistant Professor. This honor was given to her based on her research activities and students evaluating her teaching. She was awarded the UTC Outstanding Faculty Research and Creative Achievement award in 2016. She has also been awarded the best researcher award in the CSE department and the College of Engineering and Computer Science in 2010, 2013, 2014, and 2015. Dr. Sartipi has been an IEEE senior member since 2016. She has been a member of the Board of Directors for the Enterprise Center, Chattanooga, Tennessee, since 2017. Since 2013, she has also been a member of the Board of Directors for Variable, Inc., Chattanooga.

Before CUIP’s inauguration as an independent center in July 2018, Dr. Sartipi represented the Smart Cities and Urban Dynamics swimlane (now graduated) of the SimCenter. The high complexity of flows and processes involved in urban systems drives the need for powerful computing systems to develop planning, design, and control strategies; SimCenter computing and storage have figured heavily into efforts in this swimlane, bolstering researchers’ ability to collect, transmit, and analyze data, and to derive information from large datasets.
amounts of data. This feature offers a look into Dr. Sartipi’s SimCenter-related work in this swimlane in FY2018, as well as a preview of her continuing work with CUIP from FY2019 onward. Though the SimCenter will not take center stage in Dr. Sartipi’s research, we hope to be able to support her work as needed.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My research is mostly in smart city applications, specifically in areas like health, mobility, and energy. I use data-driven approaches to these areas in the local community and beyond. Health innovations include remote patient monitoring, telemedicine, data-based public health interventions, and integrated patient management systems that can significantly impact quality of life and long-term health outcomes. Other examples include advances in Vehicle-to-Vehicle Communication (V2V), Vehicle-to-Infrastructure Communication (V2I), and smart grid technology.

How did the SimCenter factor into your work in FY2018?

We have used the high-performance computing (HPC) capabilities at the SimCenter for our NSF-funded project on connected autonomous vehicles. Data collected by our vehicles was sent to the SimCenter via fiber, and the data was processed there. Results were then sent back to the vehicles to inform future iterations of design, testing, and deployment.

What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

In FY2018, we were introduced to IBM and Hexagon through Dr. Tony Skjellum, the SimCenter director. No project was initiated, but we may pursue this connection in the future.

How did you include students in your (SimCenter-related) research in FY2018?

My students were funded by external support, but one postdoc was partially supported through a CEACSE grant in which we worked on communications for smart city applications. This project, titled “Enabling Wireless 3C Technologies for Smart and Connected Cities,” investigated enabling wireless 3C (Communication, Computing, and Caching) technologies. We studied (1) 3C service deployment, placement, and migration; (2) big data-driven 3C optimization and control; and (3) 3C potential for large-scale connected autonomous vehicles in smart & connected cities.

What are your plans for continued SimCenter-related research in FY2019 and beyond?

Though CUIP is an independent center with its own research trajectory, I anticipate continuing some level of partnership as needed. I plan to continue to use the HPC and storage capabilities of the SimCenter to support CUIP research. In addition to data-driven approaches that CUIP researchers will apply to smart-city projects, we may also require simulation and modeling expertise of the SimCenter.
Dr. Eleni Panagiotou is a new Assistant Professor in the Mathematics Department. Though she did not formally begin employment at UTC until August 2018, she began making connections with the SimCenter at the end of FY2018 and will continue to build her research with SimCenter support moving forward. She received her diploma in Applied Mathematics and Physical Sciences in 2007, her M.Sc. in Applied Mathematics in 2008, and her Ph.D. in Mathematics in 2013, all from National Technical University of Athens, Athens, Greece. She previously held positions as a Visiting Researcher at ETH, Zurich, and a Visiting Assistant Professor and Visiting Lecturer at the University of California Santa Barbara (UCSB). Dr. Panagiotou's research interests are in computational mathematics and materials modeling, particularly in protein folding, topological entanglement, and polymers. She also has an established history of undergraduate research support in applied and computational mathematics.

Dr. Panagiotou’s work represents multiple swimlanes of SimCenter research, including Additive & Advanced Manufacturing and Health & Biological Systems. The latter is most prominent, and her work fits into the efforts to innovate across a wide range of bioinformatics and statistical data analysis tasks in the areas of genomics, metagenomics, transcriptomics, proteomics, epidemiological studies and electronic health record data mining. This feature offers a look into Dr. Panagiotou’s SimCenter-related research in her first few months at the SimCenter, as well as a preview of her continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My research in 2018 has been focused on undertaking two new directions in my research. First, I have been studying the relationship between topology/geometry and protein folding kinetics. These applications are different from my previous work on polymer entanglement, which was focused on polymer melts and solutions and the effects of entanglement on material properties. Because proteins are active macromolecules, their kinetics are more complicated and require more advanced computing resources, such as those available at the SimCenter. This work is in collaboration with Dr. Kevin Plaxco from the Department of Chemistry and Center of Bioengineering at UCSB.

My second, independent direction has involved studying field theoretic simulation methods and using them to detect phase transitions in polymer melts. These simulations are very different than molecular dynamics simulations. They allow simulation at much longer time scales at the cost of losing detailed molecular conformations. This work is in collaboration with Drs. Glenn Fredrickson and Kris Delaney from the Department of Chemical Engineering and the Material Science Laboratory at UCSB.

Additionally, I have worked with Dr. Ken Millet, Department of Mathematics, UCSB, on a study of classification of conformations of proteins using a new tool called the linking fingerprint.

How did the SimCenter factor into your work in FY2018?

Through the SimCenter, I applied for a CEACSE grant as a PI, with co-PIs from the Department of Mathematics and the Department of Chemistry. The SimCenter has also provided an office, a PC, and technical assistance, which I
have used to continue my ongoing work. Also, the SimCenter has co-funded the visit of Dr. Millett, with whom I am working on the classification of protein structures. In addition, the SimCenter has co-funded my conference participations. I have given invited talks at the AMS Fall Western Sectional meeting, Special Session on Mathematical Methods for the study of the Three-Dimensional Structure of Biopolymers (talk entitled “A topological model for protein folding”) and the AMS Fall Southern Sectional meeting, Special Session on The Geometry of Curves and Applications (talk entitled “The effect of topological and geometrical constraints on polymer material properties”).

Since I have arrived at UTC, in the Department of Mathematics and the SimCenter, I have written and submitted two manuscripts for publication, and I intend to use my SimCenter connections to further contribute more publications and conference talks in the coming year.

**What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?**

So far, the SimCenter has largely helped continue my previous collaborative projects. SimCenter staff have also been indispensable in helping organize talks, giving advice on grant proposals, and setting up and troubleshooting technology.

**How did you include students in your (SimCenter-related) research in FY2018?**

I am very much looking forward to continuing to work with students on research projects, as I did in the past and hope to do in the coming year. Since I arrived at UTC, I have encouraged student participation in all public SimCenter events, and some of my students have already attended the SimCenter-Math joint seminars.

**What are your plans for continued SimCenter-related research in FY2019 and beyond?**

I intend to continue my research on SimCenter-related areas, invite distinguished scientists to give talks, and apply for external funding. Also, I intend to collaborate with faculty from the Department of Mathematics and the Department of Chemistry at UTC. For my research, it is very important to continue using the computational support and high-performance computing expertise provided by the SimCenter.
DR. T. DANIEL LOVELESS is a UC Foundation Assistant Professor of Electrical Engineering (EE) at UTC. He received a B.S. degree in EE from Georgia Institute of Technology, Atlanta, Georgia, in 2004 and M.S. and Ph.D. degrees in EE from Vanderbilt University, Nashville, Tennessee, in 2007 and 2009, respectively. Prior to joining UTC in 2014, he was a senior engineer and Research Assistant Professor at the Institute for Space and Defense Electronics (ISDE) at Vanderbilt University.

Dr. Loveless has served as PI, Co-PI, or technical lead on programs totaling over $3 million in support. His research interests include radiation effects and reliability in electronic and photonic integrated circuits (ICs); high-performance and radiation-hardened digital, mixed-signal, and analog integrated circuit design; and embedded systems. Dr. Loveless has published 90 articles in peer-reviewed journals, has been cited over 1400 times, and is a Senior Member of IEEE.

Dr. Loveless is a representative of the Energy & Environment swimlane at the SimCenter, whose goal is to address challenges in energy production, vehicle technology, climate change impacts, and urban systems. For example, computational approaches and methods are revolutionizing the development of new materials while advancing our understanding of dynamic processes at the molecular and atomic level. This feature outlines how the SimCenter has supported Dr. Loveless's work.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My work has primarily tackled questions related to microelectronics reliability and the effects of space radiation on microelectronics and embedded systems. Of note, we have recently developed a spectroscopy technique that couples in situ measurements with machine learning for measurement and detection of ionizing radiation events and degradation from environmental conditions. This allows for improved reliability and operational health assessment due to the ability to handle simultaneous input constraints, e.g., elevated temperature, exposure to ionizing radiation, and over-voltage stressing. The Ionizing Radiation Spectroscopy Technique, or IRES, was a result of collaboration between Dr. Donald Reising and myself via funding from the CEACSE program, collaboration with Vanderbilt University Institute for Space and Defense Electronics, and funding from the Defense Threat Reduction Agency (DTRA).

Second, my work on radiation effects in electronics has expanded to include investigation of radiation effects in photonic devices. With funding from DTRA, we investigated the interactions of radiation with photonic ICs and optical interconnect systems through simulation of the effects of low- and high-temperature extremes and ionizing radiation on optical metamaterial-silicon interfaces.

I have also focused on implementing a Research Experience for Undergraduates (REU) program. The NSF-funded REU “UTChattSat: A CubeSat Research and STEM Program at UT Chattanooga” is a 10-week research internship at UTC. The 3-year program will accept the first cohort of ten students during the summer of 2019. Students will work closely with their mentors on cutting-edge projects in space systems, electronics, communications, and other exciting research areas. The program will specifically address research related to small satellite (CubeSat) systems, the electronics of which were developed in my research laboratory. This technology has been leveraged to develop other SimCenter collaborations in Internet of Things (IoT) and energy.

How did the SimCenter factor into your work in FY2018?

The SimCenter has provided a foundation on which I have been able to further build my seed projects to be competitive in an international landscape. Through CEACSE awards, the SimCenter has supported development of initial ideas, provided personnel for proposal development, and provided facilities to conduct research.

Specifically, we have been able to create a niche program based upon Ionizing Radiation Effects modeling. This work has resulted in extramural funding, new collaborations with...
university (Vanderbilt University), national laboratory (Sandia National Lab, Air Force Research Labs), and industry partners (Nu-Trek, Inc., Northrop Grumman). Further, much of the work conducted in FY2018 was computational in nature and required use of the SimCenter's computing capabilities, without which the work would not be possible.

What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

I collaborate closely with Dr. Donald Reising. Our work on RF-DNA fingerprinting led to a CEACSE project, titled “Unlocking the Secrets of RF-DNA Fingerprinting,” on electronics reliability, from which we developed the IRES method. In addition, we collaborate on IoT, energy, and communications projects. During FY2018, we proposed the design for an IoT Smart Buildings Laboratory at the SimCenter. Some of our early CEACSE-supported work led to the development of an Energy Assessment model with low-cost aftermarket sensors. We are in the process of developing an interactive laboratory to continue advancement in this area and enable growth in other areas. Other collaborators include Drs. Sartipi and Kandah in smart cities, wireless communication, and networks.

In addition, I continue to leverage support, computing tools, and computational expertise from SimCenter staff. Most notable are Kim Sapp, who has assisted me on many occasions and organized professional meetings and visitors on my behalf; Dr. Ethan Hereth, who has enabled my research to progress through technical support and the development and maintenance of enabling technology; and Bailey Cundiff, who has provided impeccable grant writing support.

How did you include students in your (SimCenter-related) research in FY2018?

In FY2018, I funded two M.S.-level students and one undergraduate EE student through a CEACSE grant. I have one other M.S.-level EE graduate student, funded from extramural dollars, who is conducting computational modeling work (Photonics) and is a regular user of the computing clusters.

What are your plans for continued SimCenter-related research in FY2019 and beyond?

Each of the above-stated projects will continue in FY2019. I will be more heavily focused on the development of the IoT laboratory and acquiring related extramural research dollars in this area, and I am not planning any new topical areas in the foreseeable future.
**DR. FRANCESCA LEASI** is an Assistant Professor in the Department of Biology, Geology, and Environmental Science. Though she did not formally begin employment at UTC until August 2018, she began making connections with the SimCenter at the end of FY2018. She received her M.S. degree in Biology and Ecology in 2002 and her Ph.D. degree in Evolutionary Biology in 2007, both from the University of Modena and Reggio Emilia, Italy. Dr. Leasi's research interests are in biodiversity and big data modeling.

Dr. Leasi is a representative of the Health & Biological Systems swimlane in the SimCenter, which includes efforts to innovate across a wide range of bioinformatics and statistical data analysis tasks in the areas of genomics, metagenomics, transcriptomics, and proteomics. This feature offers a look into Dr. Leasi's SimCenter-related work in this swimlane in her first few months at UTC, as well as a preview of her continuing work from FY2019 onward.

**What was your main research focus in FY2018, whether connected to the SimCenter or not?**

My research has focused on investigating biodiversity and biodiversity shifting in aquatic ecosystems. I have investigated the biodiversity of meiofauna by integrating morphology-based taxonomy, population genetics, and environmental DNA analyses. Finally, I statistically investigated correlations between biodiversity estimates and environmental parameters to formulate ecological conclusions. My main goal in 2018 has been to understand whether the biodiversity assessment method applied might bias values of biodiversity estimates and, consequently, ecological conclusions.

**How did the SimCenter factor into your work in FY2018?**

Besides access to a supercomputer, necessary for my projects based on big datasets, the SimCenter allows me to connect with faculty from other disciplines, such as environmental modelers, biostatisticians, computer scientists, and computational biologists. I received an early-faculty career grant (mini-CEACSE) offered by the SimCenter that was funded prior to the beginning of my faculty position, which allowed me to immediately connect with other faculty and start organizing my research.

**What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?**

I have collaborated with statisticians and computer scientists from other institutions, but I have never had the chance to integrate results into complex models. With the help of the SimCenter, I connected with faculty from the Civil and Chemical Engineering Department who are interested in my research ideas and started fruitful long-term collaborations that I expect will provide high-quality results.

**How did you include students in your (SimCenter-related) research in FY2018?**

I haven't had the chance to include students at UTC; however, I plan to include both undergraduate and graduate students starting in Spring 2019. Students will be involved in data acquisition and analysis, as well as presentation of results. I plan to establish interdisciplinary projects that allow students from different programs to connect, collaborate, and achieve common goals. Specifically, I plan to recruit students from the Biology, Geology, and Environmental Science; Mathematics; Computer Science; and Engineering departments.

**What are your plans for continued SimCenter-related research in FY2019 and beyond?**

I aim to use the computational resources and collaborate with faculty associated with the SimCenter. This collaboration is fundamental in a fast-changing world that requires research producing big data and data analysis using sophisticated and diverse computational tools.
DR. HONG QIN is an Associate Professor in the Department of Computer Science and Engineering and the Department of Biology, Geology, and Environmental Science. He received his B.S. in Biological Sciences and Biotechnology in 1991 and his M.S. in Biophysics in 1994, both from Tsinghua University, China; his Ph.D. in Biochemistry and Molecular Biology from the University of Chicago in 2000; and an M.S. in Computer Science from Loyola University of Chicago in 2002. Dr. Qin’s areas of expertise are graph reliability modeling, bioinformatics, computational genomics, mathematical modeling, systems biology, cellular aging, and gene network analysis and modeling, and his research represents the Health & Biological Systems swimlane of SimCenter Research. This feature offers a look into Dr. Qin’s SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

In FY2018, my group focused on developing new models and algorithms to investigate biological networks and bioimage big data. We proposed a new recursive algorithm to perform network permutations for large biological networks with power-law features. We applied this new algorithm to detect organizational patterns in cellular networks for cellular aging and tumorigenesis. In collaboration with Drs. Yu Liang, Craig Tanis, and Joey Shaw, I am developing a deep learning approach to analyzing bioimage big data, such as time-lapsed microscopic images and digitized herbarium images.

How did the SimCenter factor into your work in FY2018?

I am the recipient of an NSF CAREER award (2015–2020) and the lead PI of an NSF Big Data Spoke award (2018–2021), both of which require the computing power of the SimCenter.

How did you include students in your (SimCenter-related) research in FY2018?

One Ph.D. student, one M.S. student, and two undergraduate student researchers in my lab are supported by my current CEACSE project, titled “Analyzing Bioimage Big Data with Deep Learning Neural Networks.”

What are your plans for continued SimCenter-related research in FY2019 and beyond?

I am applying for external research funds for projects that use computational and mathematical approaches to investigate biomedical and biological questions. One focus is to develop probabilistic gene network models to infer network changes during cellular aging. Another is to develop machine learning methods to automatically estimate cellular lifespan from time-lapsed images and apply engineering principles to study molecular, biological, and ecological networks. Finally, I hope to continue to develop deep learning methods for better classification and prediction with heterogeneous biomedical and biological large data sets.
Dr. Craig Tanis is an Assistant Professor in the Department of Computer Science and Engineering. He received his B.S.E in Computer Engineering and M.S. in Computer Science from Tulane University in 1997 and 1998, respectively. He received his Ph.D. in Computational Engineering from UTC in 2013. He was awarded Departmental Teacher of the Year in 2011, 2012, 2013, and 2014. Dr. Tanis researches the use of programming language techniques in HPC, helping application scientists develop correct codes without compromising computational efficiency.

Dr. Tanis’s work represents the High-Performance Computing and Algorithms swimlane in the SimCenter, which he will lead beginning in FY2019. His work fits into the use of super computers and parallel processing techniques for solving complex computational problems, with a focus on developing parallel processing algorithms and systems. This feature offers a look into Dr. Tanis’s SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My main research has been in performance portability of a finite element code for the “PETTT: Heterogeneous HPC for High-order Stabilized Finite-elements on Moving and Deforming Domains” and “Reusable Hypersonic Vehicle Structures” projects. This work has been known in previous iterations as “The Porting of FUNSAFE from Fortran to C++,” research that enables FUNSAFE on heterogeneous systems. I have also recently become interested in distributed deep learning and video processing.

How did the SimCenter factor into your work in FY2018?

The above-mentioned projects are inherently HPC projects, and I use SimCenter resources almost exclusively for my development and testing. In particular, the TS/Oneseventeen server has been my primary testbed for this new version of FUNSAFE. I try to spend half my week in the SimCenter building to benefit from direct interaction with other SimCenter users and administrators.

What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

This FUNSAFE project is based on an extended collaboration with Drs. Kidambi Sreenivas, James Newman, and Robert Webster. I’m also on a second consecutive CEACSE award with Dr. Hong Qin, called “Analyzing Bioimage Big Data with Deep Learning Neural Networks.”

How did you include students in your (SimCenter-related) research in FY2018?

FY2018 did not offer many opportunities for students in my research, but I am moving toward more student involvement now. I have one undergraduate student working on a DHON (Departmental Honors) in deep learning and video processing. Similarly, I have a class of Ph.D. students working on applying HPC concepts to their personal research.

What are your plans for continued SimCenter-related research in FY2019 and beyond?

The FUNSAFE work will continue, but I am interested in working with more architectures from a performance portability standpoint. We are doing some preliminary work with ARM architectures and ARM+GPU systems, and I hope to do more with applications of FPGA to HPC.
DR. KIDAMBI SREENIVAS is an Associate Professor in Mechanical Engineering. He received his B.Tech. in Aerospace Engineering from the Indian Institute of Technology, Madras, India, in 2001, as well as his M.S. degree in Aerospace Engineering and Ph.D. degree in Engineering at Mississippi State University in 2003 and 2006, respectively. He pioneered the capability to enable rotating machinery simulations using unstructured meshes and has worked closely with researchers from NASA, the US Navy, the DOE, and various private companies.

Dr. Sreenivas’s work represents the Aerospace & Defense Simulation swimlane in the SimCenter, specifically utilizing modeling and simulation for evaluating and designing vehicle and weapons technology, enabling world-class aero/propulsion research, fostering science-driven technology innovation, and developing methods and tools for digital system simulations. This feature offers a look into Dr. Sreenivas’ SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

**What was your main research focus in FY2018, whether connected to the SimCenter or not?**

My research focused on (1) porting of FUNSAFE to hybrid architectures, (2) evacuation of mega cities, (3) directing undergraduate students on the Design/Build/Fly team, (4) further development of FUNSAFE, (5) working with SmartTruck on drag reduction devices, (6) working with Pointwise on grid deformation strategies for high-order meshes, (7) working with undergraduate students on various applications of Tenasi, and (8) research into river flows.

**How did the SimCenter factor into your work in FY2018?**

Most of my work utilizes SimCenter resources (papertape and oneseventeen clusters) in addition to grid generation (Pointwise), compilers (Intel), and flow visualization software (Fieldview, TecPlot). Even the research that is not directly related to the SimCenter, like the Design/Build/Fly team, will be using SimCenter resources for design simulation. The UTC Rocket Mocs (the rocket team) has also utilized Tenasi to simulate the flow around their designs and SimCenter resources were used for that purpose.

**What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?**

I am, as a result of the SimCenter’s commitment to facilitating collaboration, working with Drs. Mina Sartipi, Craig Tanis, Robert Webster, James Newman, Tony Skjellum, and Jejal Bathi. All of these are continuing partnerships.

**How did you include students in your (SimCenter-related) research in FY2018?**

I have three students working with me on SimCenter-related research. One of them is a DHON project, and the second is being funded through the Honors College. The third one is related to a workshop (organized by AIAA) we participated in back in July. The students have learned how to generate meshes and are learning to use Tenasi to solve the problems of interest.

**What are your plans for continued SimCenter-related research in FY2019 and beyond?**

I plan to continue the activities from this year. My current projects run into 2019 and beyond. Additional research aimed at porting Tenasi and FUNSAFE to ARM-based architectures will ramp up in 2019.
DR. FARAH KANDAH is a UC Foundation Associate Professor in the Computer Science and Engineering (CSE) department at UTC. He received his B.S. in Computer Science from the Hashemite University, Jordan, in 2002, his M.S. degree in Computer Science from the University of Jordan in 2005, and his Ph.D. in Computer Science from North Dakota State University in 2012. His research interests and expertise span a wide range of topics in cyber-security and cyber-physical systems networking from stationary wireless networks to ad hoc mobile networks. He is currently leading the Network Communication Laboratory (NCL). Dr. Kandah’s work represents both the Cybersecurity & Cyber-physical Systems and Smart Cities & Urban Dynamics swimlanes of SimCenter research. This feature offers a look into Dr. Kandah’s SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

Part of my focus was creating a dynamic solution using Software-Defined Networking (SDN) to meet network needs in supporting high traffic demand. We worked on developing a smart and adaptable network design that utilizes network resources more efficiently by identifying traffic patterns and analyzing network metrics to dynamically build virtual slices. With this design, we were able to minimize packet loss, maximize network link utilization, and efficiently reduce the load on the controller.

How did the SimCenter factor into your work in FY2018?

SimCenter personnel were very helpful in providing us a space to set up our experiment and giving us feedback on how to bring our research to the next level. To support the SimCenter efforts in Urban Dynamics, our team worked on developing an SDN testbed as a proof of concept that can be adopted on a larger scale. I also participated in a CEACSE-funded project titled “Enabling Wireless 3C Technologies for Smart and Connected Cities,” which investigated enabling wireless 3C (Communication, Computing, and Caching) technologies. We studied (1) 3C service deployment, placement, and migration; (2) big data-driven 3C optimization and control; and (3) 3C potential for large-scale connected autonomous vehicles in smart & connected cities.

What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

I was able to begin collaborations with faculty from Auburn University, with whom I submitted an NSF proposal to the Cyber-Physical Systems program. Though it was not funded, we plan to resubmit the proposal to another NSF program in FY2019.

How did you include students in your (SimCenter-related) research in FY2018?

Students were fully engaged in the SDN project through writing simulation experiments, building a physical testbed in the lab, and running experiments to evaluate performance of proposed algorithms and schemes.

What are your plans for continued SimCenter-related research in FY2019 and beyond?

In the future, the plan is to extend our expertise through exploring new areas in the field of Cyber-security and computer networks, as well as seeking collaborations to develop new ideas and findings. SDN, in particular, can be applied in any smart city setup to support the high demand traffic coming from different smart city entities.
DR. DONALD R. REISING is an Assistant Professor of Electrical Engineering. He received his B.S. degree in Electrical Engineering from the University of Cincinnati in 2006. He received his M.S.E.E. and Ph.D. in Electrical Engineering from the Air Force Institute of Technology in 2009 and 2012, respectively. His research interests include wireless device discrimination using RF-DNA fingerprints, digital communications, digital signal processing, and compressive sensing, which represents the Cybersecurity & Cyber-physical Systems and Energy & Environment swimlanes of SimCenter research.

This feature offers a look into Dr. Reising’s SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

**What was your main research focus in FY2018, whether connected to the SimCenter or not?**

My research has been focused on three areas: smart buildings, IoT security, and power grid resiliency. The first is a continuation of my FY2016 CEACSE grant in which I investigated the determination of energy consumption using real-time sensor measurements.

The IoT security efforts will leverage the smart building’s IoT infrastructure and looks to investigate the effectiveness of Specific Emitter Identification (SEI) in IoT security. The goal is to integrate SEI within an operational IoT network.

My ongoing work on power grid resiliency looks into the development of a hierarchical approach by which to identify electrical disturbance waveforms using machine learning. Electric Power Board currently analyzes all of this data by hand; thus, they can only process roughly 2% of all the data that is collected. My research intends to automate and improve the efficacy of this process.

**How did the SimCenter factor into your work in FY2018?**

I submitted a DARPA proposal that would have directly leveraged SimCenter resources. Also, the SimCenter is directly related to my first two efforts described above.

**What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?**

The SimCenter can play an indirect role within the last area as well through personnel connections with ORNL. I continued my collaboration with Dr. Mina Sartipi and have also started collaborating with Dr. Lakmali Weersena due to Dr. Tony Skjellum’s introduction.

**How did you include students in your (SimCenter-related) research in FY2018?**

We hired an undergraduate to continue the FY2016 CEACSE grant research. Specifically, this student made the steady-state and transient-based approach more robust to facilitate a greater number of measurements as well as sensors. This student also constructed additional sensors and developed a test plan for the validation of our developed approach using ORNL’s environmentally controlled test facility.

**What are your plans for continued SimCenter-related research in FY2019 and beyond?**

The next step in smart buildings research is to create a smart building at UTC for further smart cities research with CUIP. Some IoT extensions include intentional enhancement of RF-DNA fingerprints to enhance identification performance. Upcoming smart grid research will enable real-time network knowledge and forecasting of more serious issues due to the ability to characterize and identify waveforms.
**DR. ABI ARABSHAHI** is a Research Professor in the Mechanical Engineering Department, but he is primarily housed in the SimCenter. He received a B.S. in Civil Engineering in 1982 and an M.S. and Ph.D. in Aerospace Engineering from Mississippi State University in 1985 and 1989, respectively. His research interests include computational fluid dynamics, unsteady viscous flow applications, and grid technologies and represent the Aerospace & Defense Simulation swimlane of SimCenter research.

This feature offers a look into Dr. Arabshahi’s SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

**What was your main research focus in FY2018, whether connected to the SimCenter or not?**

My research focus has entailed the development, verification, and application of unsteady compressible and incompressible algorithms. Another focus of my research was to explore the use of a three-dimensional computational flow solver in simulation/studying of the fluid flow behavior and nanoparticles transport and deposition through different tube shapes and conditions.

**How did the SimCenter factor into your work in FY2018? What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?**

The SimCenter’s computational capabilities for simulating hypersonic flows have put me in the position to be part of a team led by the University of Dayton Research Institute for research and development of materials and structures for reusable hypersonic vehicles that travel at speeds greater than five times the speed of sound. Additionally, my collaboration with Dr. Palchoudhury has added a focus on development of a computational model for nanoparticles in the human respiratory system.

**How did you include students in your (SimCenter-related) research in FY2018?**

I mentored and advised undergraduate and graduate students involved in research associated with the SimCenter, including both monitoring the students’ progress and instructing them in using and implementing numerical grid generation software, conducting flow simulations, and analyzing the results for their projects.

**What are your plans for continued SimCenter-related research in FY2019 and beyond?**

I plan to enhance the applicability of the in-house flow solver to a wide range of problems and to continue my existing research works on the development of a higher-order accurate incompressible flow solver for studying the airflow behavior and particle transport and deposition in the pulmonary airways.
DR. SOUBANTIKA PALCHOUDHURY is an Assistant Professor in the Civil and Chemical Engineering department. She received her B.S. from the National Institute of Technology in Durgapur, India, in 2008, and her M.S. and Ph.D. at the University of Alabama in 2010 and 2012, respectively (all three in Chemical Engineering). Dr. Palchoudhury’s areas of interest include nanochemistry, biohybrid nanoarchitectures, semiconductor nanocrystals for photovoltaics, environmental nanoscience, and material characterization, especially transmission and scanning electron microscopy, which represent the Health & Biological Systems swimlane of the SimCenter.

This feature offers a look into Dr. Palchoudhury’s SimCenter-related research in FY2018, as well as a preview of her continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My research focus is to develop new nanoscale and bio-hybrid architectures for drug delivery, energy materials, and environmental applications. My research interfaces between chemical engineering, materials science, semiconductor physics, chemistry, and biology to synthesize the new nanostructures and understand their structure-property relations for different applications.

How did the SimCenter factor into your work in FY2018?

One of my main research projects in FY2018 has been to understand the flow profile of a new nanodrug designed in our chemical engineering laboratory. I was able to add a new direction to my research through my collaboration with Dr. Arabshahi with a combination of computational fluid dynamics and experimental nanoscience. Our approach was to develop a new in vitro method to determine flow of nanoscale drugs inside the body through a combination of experimental and computational flow analyses. Existing methods rely heavily on animal testing, which may not be representative of actual human body conditions.

Our collaborations have resulted in one article publication and three conference presentations.

What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

In addition to the collaborations described above, I have also established three new external collaborations with Dr. Katherine Jungjohann at Sandia National Laboratories, Dr. Nirupam Aich at the University of Buffalo, and Cellink based on my research project with the SimCenter.

What is your plan for continued SimCenter-related research in FY2019 and beyond?

I plan to investigate the flow of nanoparticle drugs through physiologically relevant biomimetic pathways in FY 2019. I also plan to use the combined computational and nanotechnology strategy to advance another emerging area in healthcare technology: point-of-care testing and diagnostics.
DR. AZAD HOSSAIN is an Assistant Professor in the Biology, Geology, and Environmental Science Department. He received his B.S. and M.S. in Geology from the University of Dhaka, Bangladesh, in 1995 and 1998, respectively, and his M.S. and Ph.D. in Geological Engineering from the University of Mississippi in 2004 and 2008, respectively. Dr. Hossain's research interests are in GIS and remote sensing, particularly in hydroscience.

Dr. Hossain's work represents the Energy & Environment swimlane of SimCenter research. His research fits into the efforts to address global, national, and regional challenges for this century by ensuring adequate supply of energy and environmental stewardship. This feature offers a look into Dr. Hossain's SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My main research focus in FY 2018 was the application of GIS, Remote Sensing, and Spatial Analysis in different terrestrial and aquatic environments using multispectral and hyperspectral remotely sensed data. Some ongoing projects include mapping urban growth using remote sensing and GIS, quantitative water quality remote sensing using multispectral and hyperspectral imagery, and application of geospatial technology in computational tools to understand the fundamental rules of life.

How did the SimCenter factor into your work in FY2018? What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

I have connected with Dr. Jejal Bathi of the Department of Civil and Chemical Engineering at UTC. We are working to integrate satellite observations with computational hydrodynamic and water quality models, and we have submitted a research proposal in response to CEACSE FY2020. This research collaboration has also created the avenue to collaborate with the National Center for Computational Hydroscience and Engineering (NCCHE) at the University of Mississippi.

Additional collaborators include Drs. Hope Klug, Jennifer Boyd, and Hong Qin for the project “Using Computational Tools to Understand the Fundamental Rules of Life”, which is currently being funded by the SimCenter, as well as Dr. Mark Schorr for research in water quality remote sensing.

What are your plans for continued SimCenter-related research in FY2019 and beyond?

I am eagerly looking forward to the proposal submitted in response to CEACSE FY2020 and plan to submit NSF and NASA ROSES proposals based on the currently funded CEACSE project. I hope to continue collaboration with Dr. Jejal Bathi and NCCHE to integrate water quality remote sensing with hydrodynamic and watershed models developed for different surface water bodies.
Dr. Jejal Reddy Bathi is a Visiting Assistant Professor in the Civil and Chemical Engineering Department. He received his B.S. in Chemical Technology from Osmania University, Hyderabad, India, in 2000; two M.S. degrees in Environmental Engineering from the National University of Singapore in 2005 and the University of Alabama in 2007; and his Ph.D. in Civil Engineering in 2008, from the University of Alabama. Dr. Bathi’s research interests are in fate and transport of nanomaterials, computational modeling of water resources, and emergency management.

Dr. Bathi’s work represents the Energy & Environment swimlane of SimCenter research. His research fits into the efforts to address global, national, and regional challenges for this century by ensuring adequate supply of energy and environmental stewardship. This feature offers a look into Dr. Bathi’s SimCenter-related research in FY2018, as well as a preview of his continuing work from FY2019 onward.

What was your main research focus in FY2018, whether connected to the SimCenter or not?

My research concentrates on developing computer-assisted simulation models to understand fate and transport of water quality parameters that are indicators of water usability and quantify available water resources under extreme weather conditions. In collaboration with SimCenter researchers, I started developing a three-dimensional hydrodynamic model that can simulate Tennessee River water quality and flooding under extreme weather conditions such as extreme droughts and 100-year floods.

How did the SimCenter factor into your work in FY2018?

I started working with SimCenter in 2017; since then, my research team has proposed use of Pointwise for developing the mesh required for our modeling work. In addition to the SimCenter hosting the license for Pointwise, Dr. Abi Arabshahi is available to provide technical support for the software.

What key research collaborations did you begin or continue in FY2018 as a result of SimCenter connections?

I have connected with several faculty, including Dr. Azad Hossain, in the Department of Biology, Geology, & Environmental Science. Dr. Hossain’s expertise in remote sensing and Geographical Information Systems (GIS), combined with my expertise in numerical watershed and hydrodynamic and water quality modeling, has led to a team that can explore applications of improved remote sensing technology in surface water quality tracking. We have submitted a proposal to the CEACSE FY2020 competition.

How did you include students in your (SimCenter-related) research in FY2018?

My research progress during FY2018 has led me develop two successful grant proposals that will fund two graduate students starting Fall 2018. The SimCenter has also offered my current graduate students working space and high-performing computers.

What are your plans for continued SimCenter-related research in FY2019 and beyond?

In FY2019 and beyond, I will expand the research begun in FY2018. In collaboration with other researchers, I have submitted three proposals to CEACSE FY2020 and two proposals to external agencies. I will continue to associate with the SimCenter to develop an interdisciplinary collaborative team to develop applied solutions for sustainable water resources.
Conference Presentations, Posters, and Proceedings

**Selected FY2018 Publications and Presentations**


J. Wang, "Computing fluid-structure interaction: from immersed boundaries to immersed domains," presented at The 5th International Conference on Modeling, Analysis, Simulations, and Applications of Inter-Facial Dynamics and FSI Problems, Sanya, China, June 2018.


**Refereed Publications**


PROPOSALS AND FUTURE GOALS

In collaboration, the College of Engineering and Computer Science (CECS), the SimCenter, and the Office of the Vice Chancellor for Research foster a rapidly expanding and enhancing culture of securing external funding as an outcome of seed research funding provided by CEACSE. We recognize the challenges for faculty to excel in attracting extramural funding while meeting all aspects of meritorious scholarship. We provide support through the Office of Research and Sponsored Programs (ORSP), through focus on opportunities that are designed to lead to larger funding awards, and through development of strategic partnerships. One new resource is the SimCenter’s recent hire of a grants administrator and technical writer. Her specific tasks include driving three CEACSE funding competitions per year and encouraging the transition from this seed funding to extramural funding by guiding faculty in proposal preparation and process management.

The 12 following SimCenter-affiliated proposals were funded in FY2018, for a total of $2,034,051.

<table>
<thead>
<tr>
<th>Title</th>
<th>PI</th>
<th>Funding Agency</th>
<th>Amount</th>
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<tr>
<td>SHF: Small: Collaborative Research: Coupling Computation and</td>
<td>Dr. Anthony Skjellum</td>
<td>NSF</td>
<td>$202,192</td>
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<td>Communication in FPGA-Enhanced Clouds and Clusters</td>
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<td>Collaborative Research: CICI: Regional: SouthEast Scientific</td>
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<td>Cybersecurity for University Research (SouthEast SECURE)</td>
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<td>Heterogeneous HPC for High-order Stabilized Finite-elements on</td>
<td>Dr. Robert Webster</td>
<td>Engility Corporation</td>
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<td>Moving and Deforming Domains</td>
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<td>Revolutionary Computational Aerosciences (RCA) Institute Support:</td>
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<td>The National Institute of Aerospace Associates</td>
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<td>Visitors and Faculty Engagement</td>
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<td>CAREER: A probabilistic gene network model of cellular aging and its</td>
<td>Dr. Hong Qin</td>
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<td>application on the conserved lifespan extension mechanisms of dietary</td>
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<td>restriction</td>
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<td>Fast Failure Recovery Methods MPI Applications</td>
<td>Dr. Anthony Skjellum</td>
<td>DOE/NNSA/LLNL</td>
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<td>Mesh curving for higher order applications</td>
<td>Dr. Kidambi Sreenivas</td>
<td>Pointwise, Inc.</td>
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<td>SHF: Medium: Collaborative Research: Next-Generation Message</td>
<td>Dr. Anthony Skjellum</td>
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<td>Passing for Parallel Programming: Resiliency, Time-to-Solution,</td>
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<td>Performance-Portability, Scalability, and QoS</td>
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<td>Reusable Hypersonic Vehicle Structures</td>
<td>Dr. James Newman</td>
<td>University of Dayton Research Institute</td>
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The 12 following SimCenter-affiliated proposals were funded in FY2018, for a total of $2,034,051.

SimCenter Awards FY14-FY18

$3,934,762

Urban Systems $878,424

Industry $1,344,000

Other $1,712,338
HANNAH GIFFORD

Hannah Gifford is a senior mechanical engineering student who just finished a minor in computer science this summer. She was originally attracted to mechanical engineering because she likes working with things she can put her hands on, and she got into computer science because she was interested in prosthetics and biomechanics. She began doing grid generation at the SimCenter last fall. Last winter, she had the opportunity to work on biomedical research with Dr. Arabshahi, simulating the movement of nanoparticles through vasculature. She has been working with Dr. Sreenivas since this spring on a validation study for simulating high-speed, subsonic flow through an S-duct for aerospace research. This study is to help assess the capabilities of current flow modeling technologies. While she is interested in aerospace research, she would love to work more in biomedical research. She will be graduating in May, and she would like to leave school and work in industry for a while rather than continuing education. She got into engineering instead of a pure science because she is more interested in working in industry than doing research, but her work at the SimCenter for UTC faculty has made her more open to graduate school and research sometime in the future. Whatever field she ends up in, she is excited to know the possibilities that simulation opens up.

STEVEN SCHMITT

Steven Schmitt received his B.S. in Computer Science: Information Security and Assurance at UTC in 2016 and will receive his Master’s degree in Cybersecurity in 2018.

His research at the SimCenter involves studying software-defined networking to leverage it in creating new security systems that use threat hunting and machine learning. His research group has created a Raspberry Pi software-defined network that they are able to use to test new ideas in the SimCenter. His general research interests include threat hunting, automated security, software-defined networking, and automated penetration testing.

He is currently employed by the federal government in cyber security and plans to continue work there to fulfill his CyberCorps obligations. After that, he plans to continue his career in cyber security either federally or in the private sector.
Aruna Doyne Saram joined the doctoral program in Computational Science with a concentration in Computational & Applied Mathematics offered jointly by the College of Engineering, Graduate School, and the Department of Mathematics at the University of Tennessee at Chattanooga (UTC) in August 2017 after finishing his M.S. in Statistics in August 2006 at Sam Houston State University in Texas and MBA with concentration in Actuarial Science at St. John’s University in New York in August 2000.

He is currently doing research under the supervision of Dr. Sumith Gunasekera. During his short university career at UTC, he has established himself as a beginner researcher in the area of Statistics and Biostatistics. His primary research area involves building and advancing Computational Statistics and Inferential Statistics, which are useful for data analysis in the areas of the Design of Experiments, Linear Models, Reliability, Availability, Survival Analysis, Statistical Distributions, etc., especially found in Pharmaceutical, Biomedical, Biometrical, Oil and Gas Exploration, Network Engineering, Engineering, Econometrical, Cybersecurity, and Agricultural research areas.

His recent involvement with the SimCenter—Center of Excellence in Applied Computational Science and Engineering (CEACSE)—made his doctoral studies, research, and dissertation stronger when his research group “CORE” (Center of Research and Exploration), headed by his mentor, Dr. Sumith Gunasekera, received the CEACSE 2018–2019 grant award in June 2018. This prompted the CORE Research group to submit another proposal for the CEACSE 2019–2020 competition. Aruna has been an active member engaging in various activities organized by the SimCenter, where he also houses his office. He strives and works hard to become a strong professorial researcher once graduated from the UTC with a Ph.D. in Computational Science with concentration of Computational & Applied Mathematics.
DR. BRUCE HILBERT graduated from UTC with three degrees: an M.Ed. in Secondary Mathematics in 2001, an M.S. in Computational Engineering in 2009, and a Ph.D. in Computational Engineering in 2015. This feature outlines his experiences with the SimCenter and how he has found them helpful in his current role.

What was your research focus at UTC?

My research was focused on computational grid generation, specifically tetrahedral grid generation: I created discrete geometries (i.e., points and lines) for use in physics simulations. I like to say I have a Ph.D. in connecting the dots...which is literally true! In addition, I was a full-time staff member at the SimCenter. My job was to generate the computational grids used in research by the faculty.

How did the SimCenter factor into your work?

As I said, I was a full-time staff member at the SimCenter, so I worked on a wide range of projects. I used commercial and SimCenter-created software to generate hundreds of computational grids for a myriad of projects including analysis of aircraft, watercraft, transfer trucks, turbomachinery, fuel cells, wind turbines, natural topographies, and nuclear reactors.

What do you do now, and how did the SimCenter help you get to where you are?

I am currently the Director of Software Engineering for Branch Technology, Inc., a startup specializing in large-scale extrusion-based fabrication, leading the programming of a unique 3D-printing algorithm. We 3D print meshes for construction and art installations. Basically, I create meshes in real-life now instead of just in the computer.

Obviously, my education at the SimCenter in meshing technology is directly relevant to my job. But, more than that, the relationships I developed there have been very important to me both personally and professionally. I was introduced to my current boss by a fellow SimCenter employee, Wally Edmondson, who is, not so coincidentally, now employed at Branch. A former advisee of mine from the SimCenter, Philip Fackler, is also employed at Branch. And my Ph.D. advisor, Steve Karman, now works for Pointwise, whose software we use in our process.

Do you have any advice for current students?

My advice is pretty simple. Work hard and take advantage of the opportunities around you. Oh, and eat lunch with your colleagues. It’s amazing how much you can learn over a sandwich.
**DR. SAGAR KAPADIA** graduated from UTC in 2008 with a Ph.D. in Computational Engineering. This feature outlines his experiences with the SimCenter and how he has found them helpful in his current role.

**What was your research focus at UTC?**

My research developed three-dimensional simulation tools to perform sensitivity analysis and design of Solid Oxide Fuel Cells (SOFCs), which are high-temperature fuel cells. When I started this topic, we didn’t have fuel cell simulation tools in the SimCenter repository, so I had to learn about fuel cells from scratch and eventually develop in-house simulation tools.

**How did the SimCenter factor into your work?**

As a Computational Engineering student, all my research work took place at the SimCenter. I was one of the lucky students who was able to extend his Ph.D. work upon graduation because I was hired as a Research Assistant Professor at SimCenter. I worked on projects such as low-temperature fuel cells (hydrogen cars), Li-Ion batteries, physics-based simulation tools, higher-order finite element methods, and data analytics. Overall, I spent a lot of time developing simulation tools for alternative energy devices.

**What do you do now, and how did the SimCenter help you get to where you are?**

I am currently a healthcare data consultant at BlueCross BlueShield of Tennessee. I spent more than ten years at the SimCenter, and, during that time, I was always working with a large amount of data and trying to make sense out of it. Though all my applications were physics based, I mastered number-crunching skills using high-performance computing. This experience has helped me immensely in my current job, as I still deal with large amounts of data and use data science techniques to make sense of it. Understanding the underlying principles of data science tools is a unique advantage I have from my SimCenter experiences.

**Do you have any advice for current students?**

Learn as much as you can. Don’t worry about the exams and understand the concepts. Once you understand the concepts, learning different technologies won’t be hard. Be a life-long student and success will follow you. Finally, become a problem solver.
HOLLEY BEELAND came to Chattanooga from the Mississippi State University NSF Engineering Research Center to join the original UTC SimCenter group in September 2002. She received her B.F.A. in Art from Mississippi State University in 1988. As the SimCenter Graphic Designer and Scientific Illustrator, Holley assists faculty and researchers in visualizing information and data generated by their research for technical proposals, manuscripts, and other applications. She also assists with web presence for the Graduate School, the Office of the Vice Chancellor for Research, URaCE, the SimCenter, Computational Science, and CEACSE.

BAILEY CUNDIFF joined UTC in March 2018. As the Grants Administrator in the SimCenter, she guides faculty in finding grant opportunities, writing and submitting proposals, and crafting strategic research trajectories; builds and maintains infrastructure to encourage improved early career faculty development and broader impacts research plans; and manages the annual CEACSE funding competitions. Bailey received her B.A. in English from Texas A&M University in 2013 and her M.A. in Technical Communication from Texas Tech University in 2017. She is currently pursuing her Ph.D. in Technical Communication and Rhetoric online at Texas Tech University.

DR. ETHAN HERETH is the High-Performance Computing Specialist at the SimCenter, a position he has held since 2016, though he has worked in other capacities at the SimCenter since 2009. Dr. Hereth received his B.S. and M.S. from the University of Central Arkansas in 2005 and 2007, respectively, and received his Ph.D. in Computational Engineering from UTC in 2016. He is in charge of designing, improving, and maintaining all SimCenter hardware, as well as installing, testing, and maintaining sundry research software spanning many application areas. His areas of expertise are CFD, MPI, HPC/Research Computing hardware, and software systems/infrastructure. In his current research, Dr. Hereth is developing automatic mesh generation software for integration of urban GIS data (building footprint data) with CFD software for the study of contaminate propagation and agent-based models.

ANNA LANE is the Budget Coordinator for the SimCenter, a position she has held since January 2018. Prior to the SimCenter, Anna was the Budget Coordinator for the UTC library, where she worked for 19 years. She monitors faculty research budgets, payroll, and other financial matters, including ledgers for funded CEACSE projects.

KIM SAPP is the Administrative Support Assistant for the SimCenter and the Computational Science Ph.D. program. She has been at the SimCenter since 2011 and earned her Certified Administrative Professional (CAP) certification in 2014. Kim coordinates travel and manages payroll for faculty, staff, and students; facilitates meetings and workshops; and offers day-to-day support for the SimCenter.