SimCenter

Center of Excellence in Applied Computational Science and Engineering

2018-2019 ANNUAL REVIEW

UNIVERSITY OF TENNESSEE CHATTANOOGA

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Bailey Kirby, Editor

Holley Beeland, Publication Design

Angela Foster (University Relations), Photography

MESSAGE FROM THE DIRECTOR

Welcome to the SimCenter Annual Report for Fiscal Year 2019 (July 1, 2018-June 30, 2019). As Director of the SimCenter, I am proud to share details of our growing capacity for research development and our growing infrastructure for scientific computing on campus.

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 PhD, 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 PhD'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 FY2019, active swimlanes included Aerospace & Defense, Cybersecurity & Cyber-physical Systems, Smart Cities, Energy & Environment, Health & Biosystems, and High-Performance Computing & Algorithms. In the final weeks of the fiscal year, we launched an additional swimlane, this one dedicated to Digital Twin technology. We will devote FY2020 to activating faculty in relevant research areas, seeking funding for concentrated research and education efforts, and accelerating workforce development in this crucial and expanding area of Industry 4.0.

SimCenter's goal is also to reach 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, machine learning, and advanced algorithms in our swimlane areas and beyond.

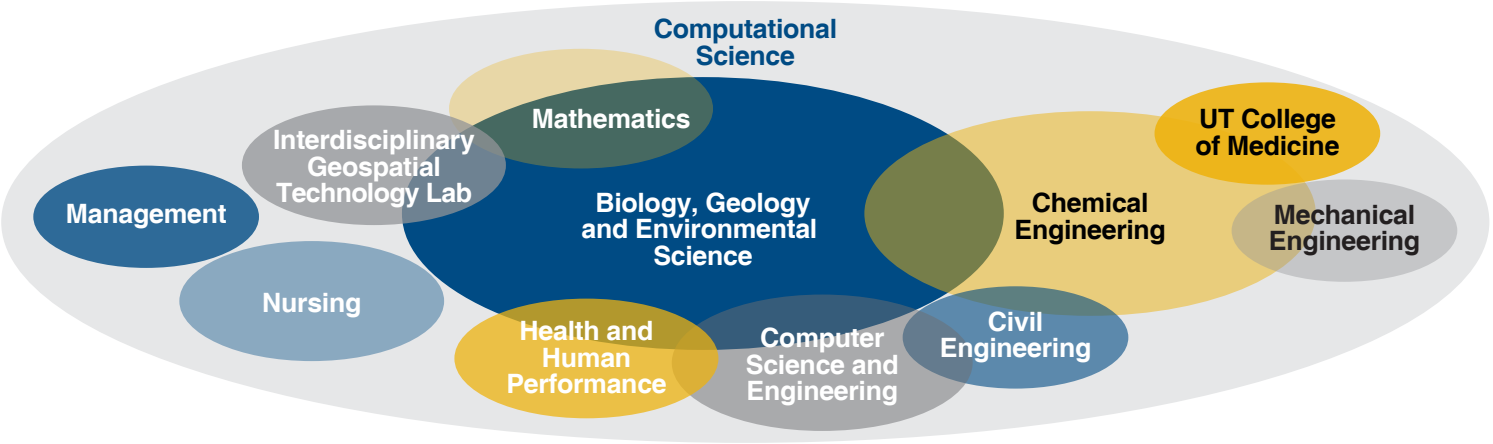
Sincerely,

DR. ANTHONY (TONY) SKJELLUM *has been the Director of the SimCenter since August 2017. He received his BS in Physics and his MS and PhD in Chemical Engineering from California Institute of Technology in 1984, 1985, and 1990, respectively. He led 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.*

SIMCENTER: UTC'S RESEARCH COLLISION SPACE

The SimCenter takes seriously its title as a state-designated Center of Excellence in Computational Science and Engineering. From the beginning, the SimCenter has been at the cutting edge of modeling and simulation research and offered technical support, computing resources, and lab/office space to exemplary faculty and students across disciplines.

Since Director Skjellum's arrival in 2017, SimCenter's efforts have expanded: retaining the emphasis on excellence in computational science and engineering, SimCenter is now the research hub for UTC at large. Faculty from across campus not only look to the SimCenter for their computing needs but also use our expertise and our space to form interdisciplinary teams with partners both on and off campus. In FY2019, we engaged 10 faculty who were new to the SimCenter, integrating them with our already robust group of core faculty. Our team-building efforts have brought together faculty in many combinations, including but not limited to the ones shown below.



Biology department chair Hope Klug has made significant progress in team-building efforts, successfully bringing together two separate groups of faculty from biology, math, computer science, mechanical engineering, and health and human sciences at UTC. Several research projects have resulted from these ongoing meetings, including grant proposals to both local foundations and federal agencies. Faculty—new faculty in particular—benefit from this arrangement by being introduced to colleagues whose research complements their own but with whom they would have never interacted otherwise. We plan to replicate this collision-space model as much as possible with other departments' areas of research.

Another successfully accelerated research group is Dr. Azad Hossain's convening of the Inaugural Workshop of Southeastern Computational and Geospatial Environmental Hydrology, a multi-institutional group he founded with the help of Dr. Mustafa Altinakar at the University of Mississippi National Center for Computational Hydroscience and Engineering (NCCHE). The attendees found common ground in their research efforts and declared a shared vision for regional collaboration on federal funding opportunities and beyond. The next workshop will be held at NCCHE during FY2020.

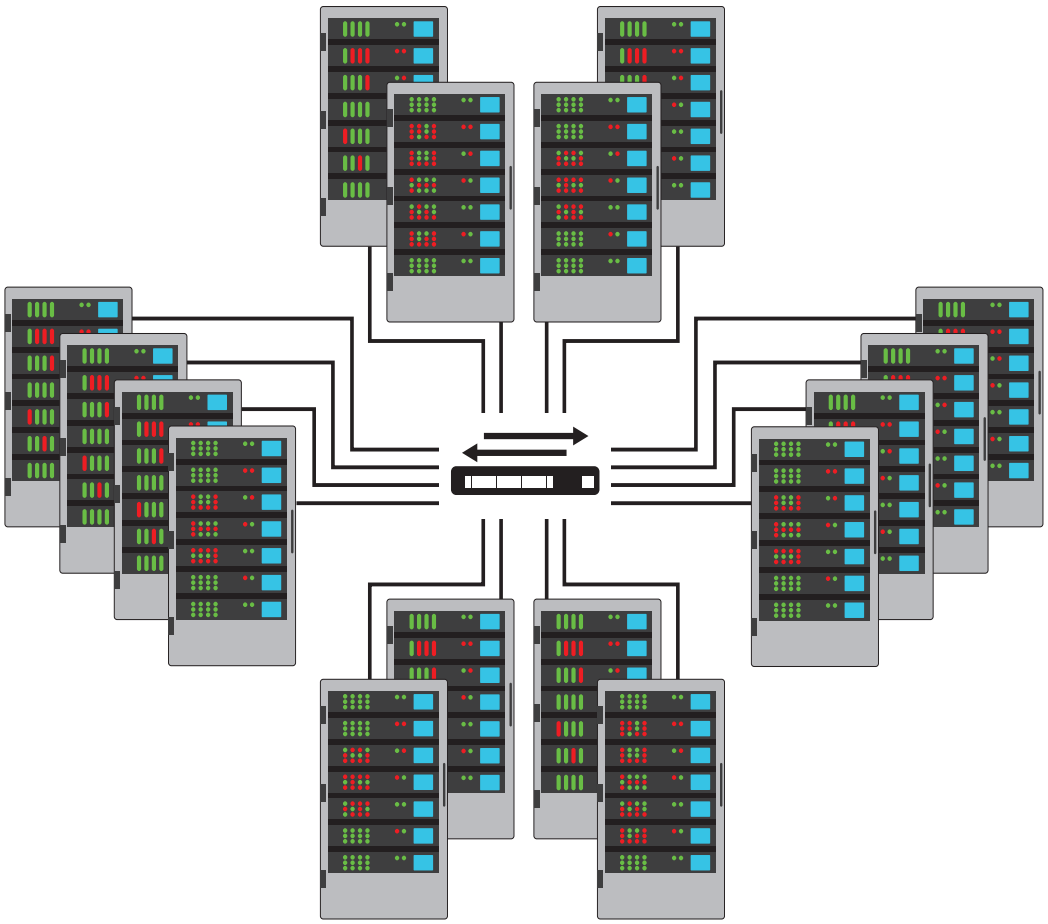
Additionally, partnerships with local small businesses, such as IMSA and Branch Technology (see p. 22), represent just the beginning of SimCenter efforts to support advances in computational science and engineering beyond the borders of UTC.

INFRASTRUCTURE IMPROVEMENTS

CC* Compute Grant: Modern High-Performance Computing Infrastructure

A team of researchers—PI Anthony Skjellum and co-PIs Ethan Hereth, Eleni Panagiotou, Kidambi Sreenivas, and Craig Tanis—won funding from the National Science Foundation this past year to effect a significant upgrade to the campus cyberinfrastructure that will provide state-of-the-art, cost-effective, high-performance computing (HPC) not previously possible. This cluster will be housed in the SimCenter data center and will significantly improve UTC's researchers' and students' ability to perform, enhance, and expand their current computationally intensive research, prototyping, and development activities and will complement other investments already made, in progress, or on the plan-of-record of UTC, including access to commercial cloud computing services. In addition to computer science and engineering, the UTC team anticipates significant research projects in mathematics, hydrology, and computational fluid dynamics that will engage four regional partner universities. Two teaching projects address HPC education and use of HPC for mechanical engineering undergraduate research/design. In addition to these funded projects, merited additional research projects are enabled over time as the PIs, Central IT, and the cluster's Advisory Board attract and onboard additional researchers and students requiring HPC. Among other users are UTC's more than 20 computational science PhD students, plus several postdocs. Furthermore, SimCenter supports undergraduate research through self-funding and Research Experience for Undergraduates in HPC, providing additional users for the proposed cluster.

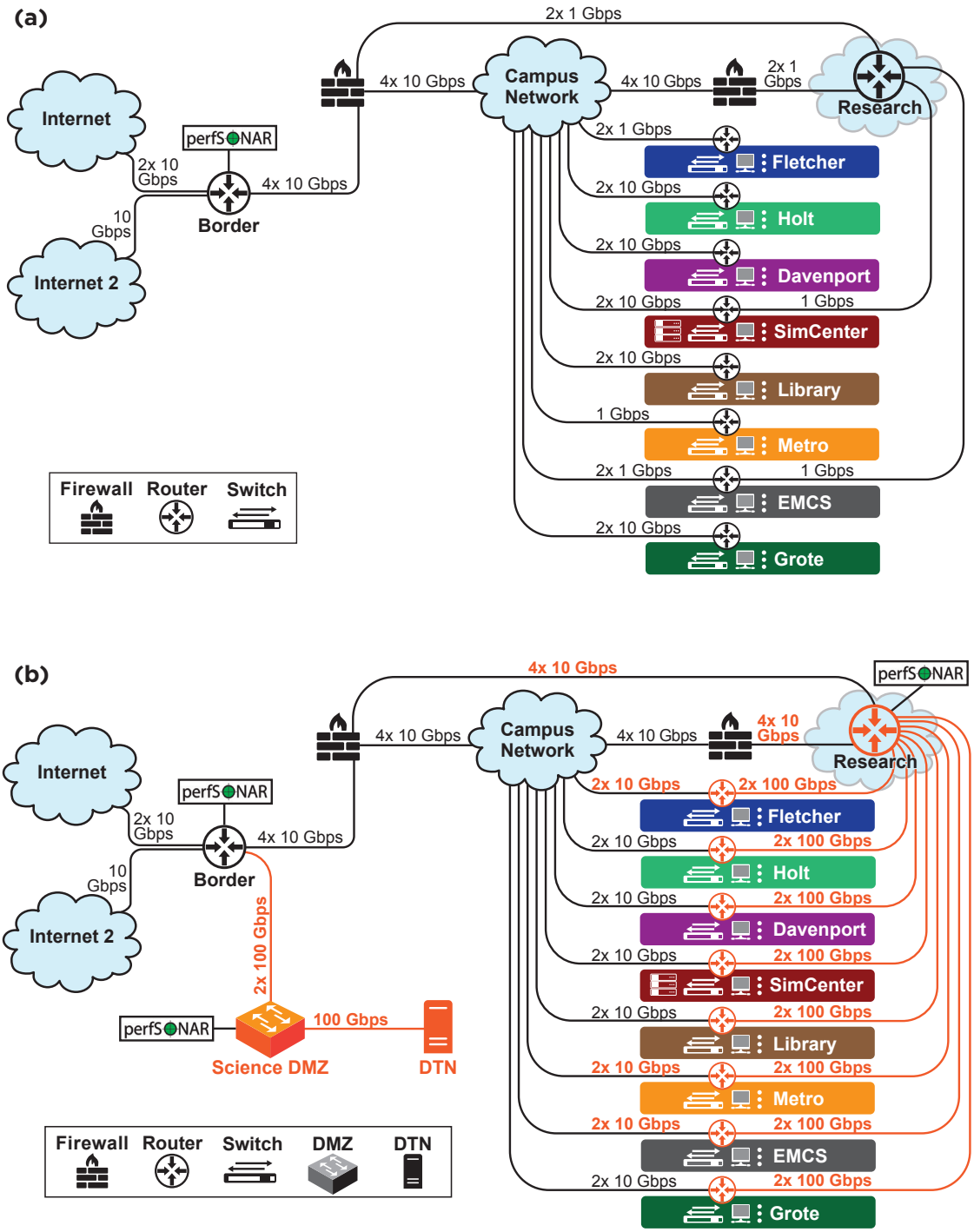
This award enables UTC to procure an innovative, 2,048-compute core, 16-server AMD EPYC2 cluster networked with 100Gbit/s InfiniBand plus 8TB of main memory and 77 Tflop/s of double-precision floating point arithmetic. EPYC2 Rome 7nm processors will be newly available on the market in Fall 2019, so this project includes state-of-the-art, cost-effective, high-performance computing not previously possible using Intel or AMD processors. The university has invested in a "commodity" cluster as recently as three years ago, and it is heavily utilized by the existing user base. That system will be nearly four years old by the beginning of this project. By way of complement, upgrades to storage (1.1PB), internal networking, data center infrastructure, and private cloud virtualization have prepared UTC to support a new campus-wide cluster with a growing number of users. The new campus cluster will enable core scales and total cluster memory not previously available on campus and thus help researchers prepare their scalable problem scenarios for greater scales on national resources such as XSEDE. Projects enabled immediately are 14 science driver projects (12 research, two teaching; see p. 6-7). Seven projects involve four regional partner universities. At least ten NSF grants at UTK, UTC, UAB, Tennessee Tech, and Ole Miss are enhanced. Project areas highlighted include fault-tolerant parallel computing, performance monitoring of HPC, next-generation parallel programming with MPI, special-purpose linear algebra, hydrology, and computational fluid dynamics research.



Concept diagram of the new campus cluster: 2,048 EPYC2 Rome cores in 16 servers connected by EDR InfiniBand. Further connection to storage, LANs, and the Internet is via IPoverIB over the same network.

CC* Networking: 100Gbit/s Research Network Connecting SimCenter to Academic Buildings

A team of UTC researchers—PI Farah Kandah and co-PIs Dennis Gendron (IT), Mina Sartipi, Hope Klug, and Tony Skjellum—is upgrading the campus network infrastructure to improve the ability of professors and students to perform, enhance, and expand R&D activities. This project complements other significant and ongoing investments/upgrades at UTC to enhance campus intra- and inter-networking and research computing cyberinfrastructure. UTC's growing research portfolio of faculty-driven, data-oriented research drives the network upgrades. 100Gbit/s fiber networking infrastructure, switching, and routing infrastructure are upgraded by this project. A Science DMZ infrastructure and Data Transfer Node (DTN) server, both components used for inter-campus collaborations and tuned for large-scale data transfers, support the emerging uses of big data and data-centric external collaborations.



Current vs. Upcoming Networking Infrastructure. New additions to the infrastructure—including eight academic buildings, many 100Gbit/s links, a DMZ, and a DTN—are highlighted in orange in part (b).

The project upgrades networking to eight UTC campus buildings representing all four university colleges (Engineering & Computer Science, Arts & Sciences, The Gary W. Rollins College of Business, and the College of Health, Education, and Professional Studies), as well as the Multidisciplinary Research Building (MDRB), SimCenter's home, and the campus library. In these buildings, at least fourteen science drivers (projects) on campus benefit from the proposed infrastructure (see p. 6-7); several of the projects are either NSF funded or otherwise externally supported. The co-location of three research centers plus UTC's research computing facilities in the SimCenter adds to the campus impact.

SCIENCE DRIVERS: RESEARCH-COMPUTING PROJECTS ON CAMPUS

To secure CC* funding—for both the campus-wide networking infrastructure and SimCenter computing cluster awards—PIs Tony Skjellum and Farah Kandah had to demonstrate buy-in from UTC faculty across disciplines. They and Grant Administrator Bailey Kirby put out a campus-wide survey that asked faculty what kinds of big data, research computing, and other relevant tasks they regularly undertake to complete their research. The results of this survey uncovered 50+ research and education projects ("science drivers") from 30+ faculty from UTC, as well as additional faculty at UTK, UAB, and TTU. These faculty spanned all four colleges at UTC—Engineering and Computer Science; Business; Arts and Sciences; and Health, Education and Professional Studies—in addition to the UTC library and IT department. See below for a selection of projects from those proposals that will be accelerated by the implementation of these two prestigious awards.

PROJECT TITLE: Smart Campus through Smart Buildings
PI: Dr. Farah Kandah, Associate Professor in Computer Science and Engineering

This project will instrument an existing room/laboratory at SimCenter with edge devices (IoT packages and gateway devices all networked to a small cloud), sensors, and experimental measurement equipment. Internal sensor/IoT packages will be designed to operate in settings using parasitic power, make minimal or no impact on existing infrastructure, and be scalable to floors and a whole building (approximately 2,000 such packages are planned). Initially, sensors will be installed to provide raw data on temperature, occupancy, lighting, and other measurable parameters and create a degree of instrumentation of a smart space not currently available to UTC researchers or to many researchers nationwide. The IoT gateways will also be expandable to include additional sensors.

PROJECT TITLE: Evolutionary Ecology Research
PI: Dr. Hope Klug, Associate Professor in Biology, Geology and Environmental Science

Predicting how genes and the environment interact to produce phenotypic traits is a fundamental question in the natural sciences. Identifying the biotic and abiotic rules that create the genotype-to-phenotype map requires that we examine patterns of biological diversity (1) across levels of biological organization and at various geographical scales, (2) in relation to interactions among the environment and in relation to ecology and evolution, and (3) across a range of species. We will use the computing resources at SimCenter to utilize existing big datasets and computational tools (e.g., network analysis) to develop and analyze biological networks of interest across species and spatial scales to identify the key interactions that influence the genotype-to-phenotype map that leads to diversity in reproductive and parental investment. We will initially focus on reproductive and parental behavior, as these behaviors are to some extent exhibited by all organisms. In the future, though, this system can be used to help identify the factors that explain diversity in a range of phenotypic traits.

PROJECT TITLE: Smart River Project
PI: Dr. Mustafa Altinakar (*left*), University of Mississippi, National Center for Computational Hydroscience and Engineering
Co-PI: Dr. Azad Hossain (*right*), UTC Assistant Professor in Biology, Geology and Environmental Science

In this project, river water quality and aquatic eco-environment will be studied and monitored using remote sensing technology, numerical modeling, and ground measurements (point sampling). Well-verified and -validated multi-dimensional surface flow, sediment transport, and water quality models will be applied for continuous and long-term simulations of different water quality and ecosystem variables in the Tennessee Rivers, including Chickamauga Lake, in near real-time. The two- and three-dimensional models developed by NCCHE will be used. Water quality and ecosystem processes in water column and bed sediment layers will be simulated. High-speed and parallel computing facilities are necessary to resolve spatial details and time evolution of these processes. In addition, computing power will be needed to visualize and analyze simulation results and to extract scientific and decision-making information for researchers and management.

PROJECT TITLE: Sport Injury Predictive Modeling and Providing a Smartphone Application to Local Athletic Trainers for Collecting Pre-participation Screening Data
PI: Dr. Gary Wilkerson, Professor in Health and Human Performance

The goal of this project is to create a smartphone app, usable by high school athletic trainers, to gather electronic data at sport pre-participation examinations to allow surveillance of injury occurrences. Predictive modeling will guide implementation of individualized injury risk-reduction training activities. Potential exists for rapid expansion of the project to include schools spread over a large geographic area. Erlanger, a major hospital system with a branch local to UTC, has the contract for providing athletic trainers to local high schools, which represents an opportunity to obtain standardized data and injury information on a large number of athletes using a smartphone application and cloud-based injury documentation software. We anticipate collecting biomechanical and injury data on 500 high school athletes and rolling this capability out to other school districts in subsequent years.

PROJECT TITLE:
Studying Knowledge-Sharing Behavior of Medical Professionals on Twitter
PI: Dr. Hemant Jain, Professor in Management

This project focuses on the social capital within implicit communities that develop on social media platforms. Specifically, it studies—based on social capital and social network theories—the engagement of healthcare professionals on Twitter. A novel data collection approach was developed to identify implicit communities and patterns of connection within the popular social media platform Twitter. Analysis of healthcare professionals' activities within the identified communities over a six-month period shows structural topology of implicit communities. The structural positions of members within the community are associated with the level of members' participation in implicit online communities.

PROJECT TITLE: FUNSAFE: A Performance-Portable, Scalable Finite-Element Code
PI: Dr. Craig Tanis, Assistant Professor in Computer Science and Engineering

FUNSAFE is a modular unstructured finite element code used for simulations based on a variety of physics models, including high-order compressible/incompressible fluid dynamics, time-domain electromagnetics, and acoustics. Developed by researchers at the UTC SimCenter, FUNSAFE exists in two forms: (1) as a mature MPI-parallel Fortran code and (2) as an experimental MPI+X C++ code based on the performance portability framework Kokkos and numeric libraries from the Trilinos suite of scientific software. The C++ version is capable of executing at multiple levels of shared and distributed parallelism, with or without computational accelerators, and is currently capable of using MPI, OpenMP, and Cuda simultaneously. FUNSAFE will be modified to exploit the 256-bit load/stores and high-performance vector units of the EPYC2 architecture, introducing a third layer of parallelism: MPI + OpenMP + AVX. This hybrid approach will lead to significant opportunities for performance analysis, with a focus on distributing and coordinating access to unstructured mesh data across the nodes.

PROJECT TITLE: Polymer Entanglement and Architecture: Effects on Material Properties and Function
PI: Dr. Eleni Panagiotou, Assistant Professor in Mathematics

By looking at macromolecules as mathematical curves in space that do not intersect, we can study their topological entanglement using tools from knot theory. Except for the difference in context, one of the main difficulties in applying tools from knot theory to polymers has been that tools of topological complexity traditionally refer to closed curves: a knot is one or more simple closed curve(s) in space without intersections. A measure of topological entanglement that is meaningful for open chains is the Gauss Linking Integral. To study the topology of polymer chains in solutions and melts, it is necessary to use 3-dimensional simulations. All the relevant computational methods (Molecular Dynamics, Self-consistent Field Theory simulations, etc.) have strengths and limitations. To gain deep understanding of the topological, physical, and chemical properties of polymers and to measure the complex, multifaceted, and multiscale entanglement effects in polymer melt mechanics, this project uses a holistic modeling and simulation framework that combines microscopic (e.g., MD simulation) and macroscopic (e.g., Field-theoretic simulation) methods, as well as integrates topological, computational, and experimental approaches.

SWIMLANES: RESEARCH FOCUS AREAS

AEROSPACE AND DEFENSE

The Aerospace and Defense swimlane, led by Dr. James Newman, has been a long-time strength of the SimCenter. This area focuses on basic and applied research within that sector, which has been at the forefront of utilizing modeling and simulation for evaluation and design of vehicle and weapons technology. SimCenter researchers contract with national government and industry agencies in aerospace and defense. Technological advancements made by SimCenter researchers are nationally recognized in high-order stabilized finite-element technology, rotating-machinery, and aerodynamics/hydrodynamics.

Within Tennessee, swimlane members have been interacting with UT Knoxville and the UT Space Institute at Tullahoma, as well as the USAF Arnold Engineering and Development Center at Tullahoma. The objectives are to enable world-class aero/propulsion research, foster science-driven technology innovation, and lead the development of methods and tools for digital system simulations.

Much of the technology and capabilities being developed within the Aerospace and Defense application area has dual-use and applicability in Energy and Environment, Health and Biological Systems, and Digital Twins swimlanes. Additionally, the use of data analytics to calibrate and build data-driven models is becoming more widespread within many areas of Aerospace and Defense.

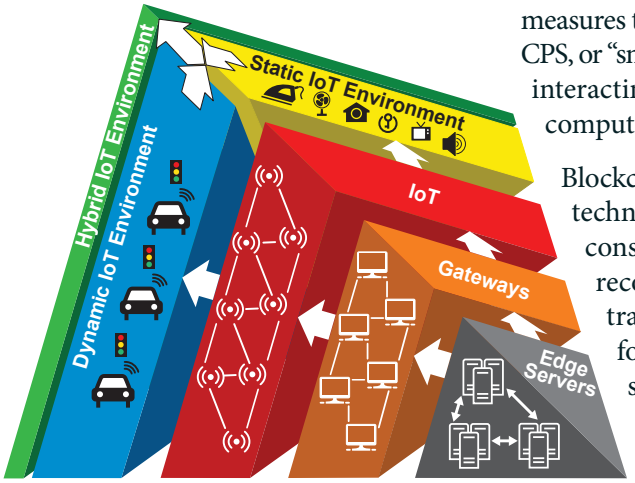
HIGH-PERFORMANCE COMPUTING AND ALGORITHMS

High-performance computing (HPC) is the use of supercomputers and parallel processing techniques for solving complex computational problems. HPC technology focuses on developing parallel processing algorithms and systems by incorporating both administration and parallel computational techniques.

The work of Dr. Craig Tanis, swimlane lead, involves performance portability, distributed deep learning, and video processing. Dr. Tanis uses the resources given at the SimCenter for his development and testing and spends most of his time there. Currently, Dr. Tanis is continuing his research on the FUNSAFE project and is encouraging more student involvement with his research.

This swimlane is additionally supported by Dr. Skjellum, as it is directly in line with his expertise and ongoing projects. Drs. Skjellum and Tanis are expanding this research thrust to include HPC education and training: they have submitted several NSF proposals to bolster all these efforts and recently won funding from NSF's Scalable Parallelism in the Extreme (SPX) program together with Boston University and Sandia National Laboratories and are looking to partner with local organizations to strengthen them.

CYBERSECURITY AND CYBER-PHYSICAL SYSTEMS



The Cybersecurity and Cyber-physical Systems (CPS) swimlane is helmed by Dr. Farah Kandah. This swimlane currently has three foci: cybersecurity, blockchain technology, and hardware-software codesign. Cybersecurity is the state of being protected against the criminal or unauthorized use of electronic data, or the measures taken to achieve this protection. CPS, or "smart" systems, are co-engineered interacting networks of physical and computational components.

Blockchain is a recent, breakthrough technology used to create a consistent, tamperproof ledger that records financial and other trans-actions without the need for a centralized "bank." In CPS, such as connected autonomous vehicles, blockchain can help construct a trust framework that adds an additional security layer, comprise a global trust-based blockchain database to support integrity and availability, and underlie a verification system with a non–computationally intensive blockchain between platoons of vehicles.

The combination of cybersecurity and blockchain with hardware-based security has led to a series of projects based on a hardware-software codesign framework developed by Drs. Farah Kandah, Tony Skjellum, Don Reising, and Daniel Loveless. RF-DNA fingerprinting is presented as a PHY layer mechanism for verifying the identity of a specific transmitter. RF-DNA fingerprints exploit the distinct and unique coloration that is imparted on the waveform during its formation and transmission. This framework works from the ground up to develop a flexible approach to CPS contexts such as both static and dynamic smart cities setups.

In 2019 and moving forward, Dr. Kandah plans to extend his expertise by discovering new areas in cybersecurity and collaborating across disciplines to grow the swimlane.

HEALTH AND BIOLOGICAL SYSTEMS

This swimlane, led by Dr. Hope Klug, is highly effective at forming collaborations with biomedical scientists from across the UTC and University of Tennessee Health Science Center's College of Medicine Chattanooga (UTCOMC) campuses to provide computational solutions for their research projects. Its goal is to position the SimCenter core capabilities and expertise as an integral part of these collaborations. With access to high-performance computing systems, health and biomedical scientists are able to perform 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.

Current partnerships associated with biomedical and biobehavioral research at UTC include the UTCOMC, UTK, UTHSC, Emory University, the American College of Sports Medicine Foundation, Vanderbilt University, Erlanger Health System, Blue Cross Blue Shield of Tennessee, TVA, Chattanooga/Hamilton County Health Department, Southeast Regional Office of the Tennessee Department of Health, and the Tennessee State Department of Health.

Recently, researchers in this area have been engaged in developing simulations of airflow and particle transport in CT-based human airway models; data analysis and modeling to predict rupture of aneurysms; simulation-based design to reduce the failure rates of percutaneous coronary interventions employing stents; analysis and design of osseointegrated dental prostheses; modeling and uncertainty quantification due to patient specific biophysical property variability for fine needle tissue electroporation and for femoral neck fractures; algorithms for index case identification and exposure prediction in infectious disease epidemics; and more.

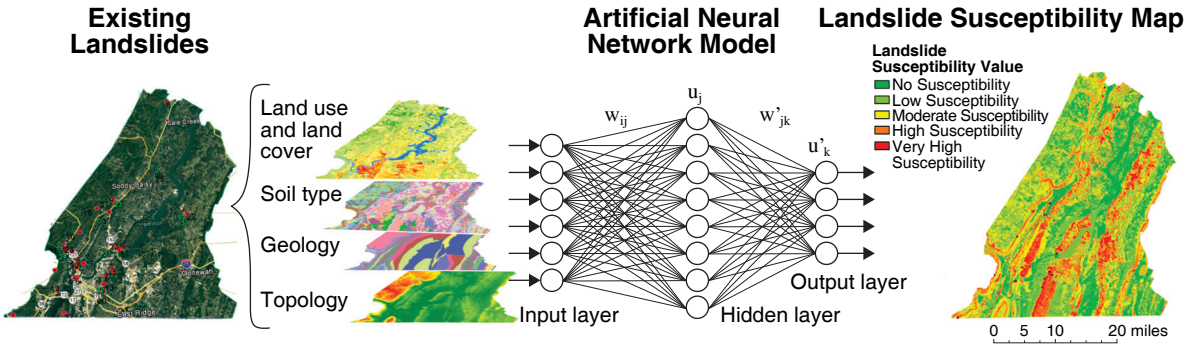
ENERGY AND THE ENVIRONMENT

ENERGY

The Energy and Environment swimlane, led by Dr. Don Reising, consists of two independent and thriving divisions. Among the defining global, national, and regional challenges for energy research is ensuring adequate supply of energy without compromising our collective ability to sustain our changing habitat as the global human population is on a path to grow from presently some seven billion to nine billion or more. Challenges in this broad area relate to energy production, transmission, storage, and efficient use; vehicle technology and transportation systems; critical infrastructures; dynamics of ecosystems, climate change impacts, adaptation, and urban systems; and others. Modeling and simulation are integral to solving many of these important problems. For example, computational approaches and methods, combined with certain analytical techniques, can handle the complexity of advanced energy transmission systems, such as the "smart grid."

This swimlane has recently focused on Dr. Reising's and others' research in smart buildings, including real-time monitoring and reporting of energy use. The main goals are to assess existing building energy models, predict energy consumption using in-situ data collection, and integrate CPS-based measurement within the building energy model. One anticipated result of this work is a functioning "smart floor" prototype in a building on UTC's campus, to later lead to a full smart building.

THE ENVIRONMENT



The other half of the Energy and Environment swimlane has two pillars: water quality and urban water resources management. The water quality pillar, based on Dr. Azad Hossain's work, is currently invested in developing a remote sensing–based algorithm to study surface water quality at watershed scales in Southeast Tennessee using satellite observations coupled with field measurements. The goal is to study impacts of land use and land cover change on the surface water quality in the watersheds of Southeast Tennessee. Additional applications include measuring stream impairment and mapping heat islands and their effect on water availability and quality. Dr. Hossain has also successfuly applied similar methods to landslide detection.

The aims of the urban water management pillar, based on Dr. Jejal Bathi's work, are to bring in integration for watershed-wide operational and informational efficiency and to develop integrated computer tool(s) that are predictive and decision-supporting. Current research emphases include surface runoff modeling and fate and transport of engineered nanomaterials.

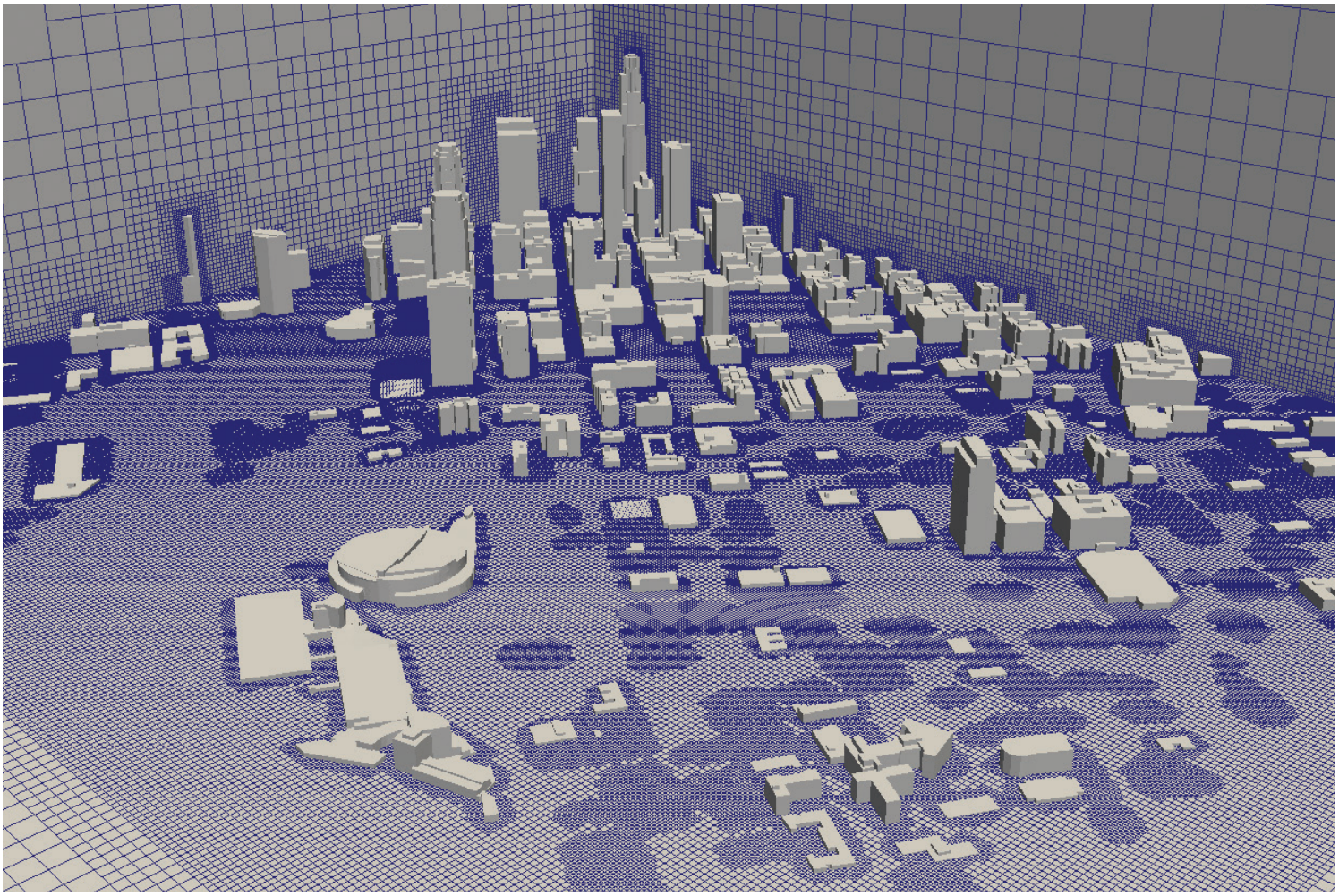
SWIMLANES: RESEARCH FOCUS AREAS (CONT.)

DIGITAL TWINS

Digital twins are software systems that facilitate the means to monitor, understand, and optimize the functions of all physical entities, living as well as non-living. In fact, it is likely that by 2021, half of large industrial companies will use digital twins. Expensive machinery, delicate parts, and complex systems can be digitally modeled in real time: paired with predictive analytics and forecast models, data collected by studying digital twins can transform a company's production capabilities. These systems are arguably as complex in their algorithms, data, and software as the physical systems they model, but they offer an effective way to mitigate risks and improve performance without significant loss of time or money. In specific applications, digital twins can be used to support model-predictive control of systems to improve safety, efficiency, profitability, and performance.

This data-driven approach to integrating online information with physical operations is a crucial driver of so-called Industry 4.0. Recent advances in overlapping fields of science and engineering, such as high-performance computing (HPC), big data, networking, and numerical modeling and simulation, are what have enabled Industry 4.0 and thus the design and application of digital twins. Because of this complexity, digital twin design, implementation, and operation are often taught and learned as separate skill sets. Those separate skill sets are then practiced by individuals from varying backgrounds and with varying levels of expertise. In a production environment, machine operators must, for instance, interface with designers and programmers. Each group has its own understanding of a digital twin system's purpose and applicability; bridging gaps in knowledge and communication between those groups is paramount to safe, effective, and efficient digital twin operation. Identification of both the skills gap and the future potential jobs needed to fill it has already begun, such as the "Digital Twin Engineer Persona" described by Deloitte in 2018.

Production engineering in Industry 4.0 in fact requires digital twins, but digital twin technology cannot mirror and pace the emerging complexity of Industry 4.0 without specialized, multidisciplinary education and workforce development with a strong foundation in software

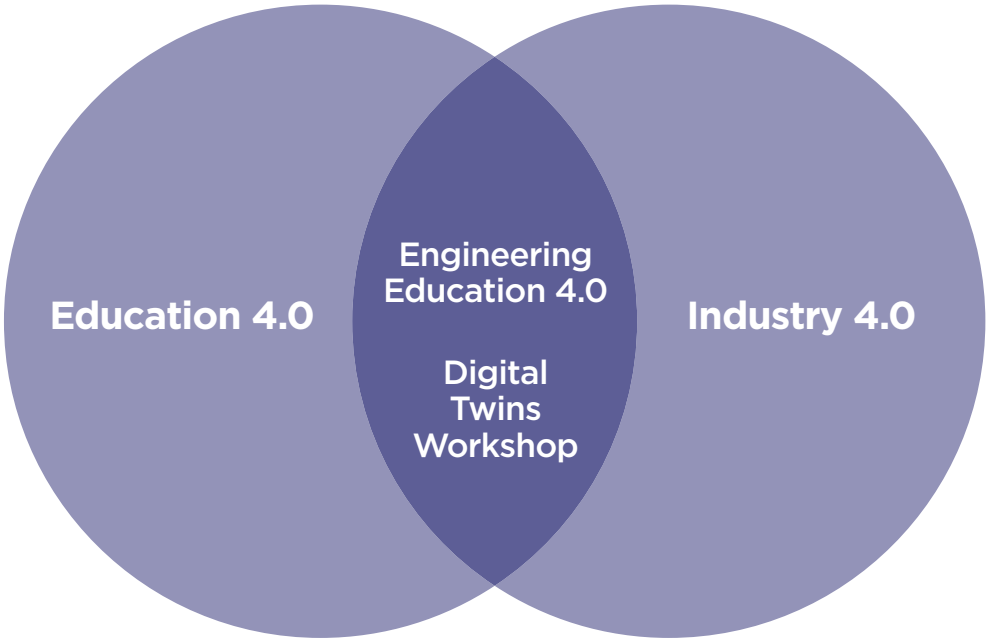


engineering. Simply put, digital twins cannot be treated as an afterthought. As industries adopt data- and technology-driven approaches to manufacturing, education must keep pace accordingly: we need knowledge workers who can reliably design, develop, and operate production-ready digital twins at a high level.

To meet this need, researchers at UTC and Tennessee Technological University (TTU) will use an FY2019 NSF award to host a pair of workforce development workshops that will convene thought leaders in multiple areas—including but not limited to engineering education, software engineering, HPC, uncertainty quantification, control systems, cybersecurity, machine learning, and cyber-physical systems/Internet of Things—to strategize educational approaches to digital twin modeling and simulation. Problems at the intersection of these disciplines are critical to achieving scalable, reliable, and cost-effective digital twins of sufficient fidelity for complex systems and production engineering, such as manufacturing and chemical plants, airplanes, and wind turbines.

The two-day workshops will focus on effective pedagogical and andragogical strategies for the intersection of Industry 4.0 and Education 4.0 via Engineering Education 4.0, using digital twins as the platform to disseminate best practices in higher education.

Education 4.0, like digital twins, is a combination of physical and virtual information. Using virtual reality in the classroom is one example; adding process management to information science curriculum is another. Accordingly, Engineering Education 4.0 encompasses engineering design challenges that result from Industry 4.0, including digitizing manufacturing. The goal of integrating digital twins into Engineering Education 4.0 is to connect theory with case studies—to help students understand the challenges of real production spaces and help employers understand the constraints of education. What's more, well-executed



digital twins (created and/or managed by knowledge workers who have been educated in the particular challenges of digital twins and Industry 4.0 via Engineering Education 4.0) can ideally be redeployed in experiential learning and workforce development.

The activities/outcomes/topics of the workshops, emphasizing digital twins workforce development at the intersection of Education 4.0 and Industry 4.0, will include the following:

- Create a roadmap for digital twin educational infrastructure for workforce development (courses, delivery modes, learning outcomes) via Engineering Education 4.0
- Identify skill sets and roles for knowledge workers who interact with digital twins in Industry 4.0
- Identify open and existing areas of research and inquiry needed to implement the educational infrastructure roadmap
- Propose transformational, cross-cutting training in HPC and systems modeling for engineers already trained in particular domain areas (e.g., vehicles, manufacturing plants, control systems)
- Identify and compile gaps in underlying disciplinary / educational areas (or uncertainty at the multidisciplinary interfaces of these areas) that limit the productive design, implementation, deployment, and utilization of digital twins for which additional R&D and educational research are needed
- Recommend strategies for the timely realization of the roadmap, such as funding mechanisms; sustained, organized collaborations of the public and private sectors with academia; and the formalization of sub-disciplines within the space of digital twin technologies

The first workshop, to be held at UTC, will elicit knowledge units to be taught at the intersection of the disciplines required to achieve production-ready digital twins. The second workshop, to be held four months later at TTU, will emphasize translation of the engineering methodologies into modules that are suitable for delivery in multiple educational formats, including both face-to-face and distributed environments for graduate and continuing education.

The digital twins swimlane is expected to grow out from these workshops, with the careful guidance of Dr. Abi Arabshahi, Research Professor in SimCenter.

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

The University of Tennessee at Chattanooga's (UTC) Center of Excellence in Applied Computational Science and Engineering (CEACSE) 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. With our previous report for FY2018, CEACSE marked its 13th 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. In FY2019, CEACSE has demonstrated a greater emphasis on its focused priority areas and achieved even greater impacts across a range of stakeholders, due not least to ongoing strengths of its visionary leadership team. 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 PhD students.

CEACSE research and advanced development activities enhance education at all academic levels at UTC including through the PhD 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. The Multidisciplinary Research Building (formerly SimCenter building), 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 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 in FY2019 include these highlights:

- Dr. Hong Qin was awarded $359,971 for the NSF project entitled "REU Site: iCompBio - Engaging Undergraduates in Interdisciplinary Computing for Biological Research."
- Dr. Abdollah Arabshahi took over an NSF project entitled "RUI†: Efficient Adaptive Backward Stochastic Differential Equation Methods for Nonlinear Filtering Problems," which remained at UTC when former UTC faculty Dr. Feng Bao relocated to Florida. The remaining award totals $124,995.
- Dr. Hong Qin was awarded $549,888 for the NSF project entitled "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education."
- Drs. Tony Skjellum, Don Reising, and Farah Kandah received $250,000 from the Oak Ridge National Lab/UT/Launch Tennessee RevV program for collaborative R&D in modeling, simulation, and engineering with International Maritime Security Associates, Inc..
- Drs. Tony Skjellum and Craig Tanis received $450,097 from the National Science Foundation for collaborative work with Boston University on Heterogeneous HPC, titled "SPX: Collaborative Research: Intelligent Communication Fabrics to Facilitate Extreme Scale Computing."
- Drs. Tony Skjellum and Craig Tanis received $100,000 from Sandia National Lab for study of Exascale Computing.
- Dr. Tony Skjellum received $60,000 from the Lawrence Livermore National Laboratory for Fault-Tolerant HPC Research.
- Dr. Farah Kandah was awarded $499,663 from the National Science Foundation for the project entitled "CC* Networking Infrastructure: Advancing High-Speed Networking at UTC for Research and Education," to support 100Gbit/s networking to connect CEACSE computing and data resources with seven other campus R&D centers, enabling modeling and simulation work and accessibility across campus. These resources are being deployed in FY2020 and FY2021.
- Dr. Tony Skjellum and team were awarded $392,235 from the National Science Foundation for "CC* Compute: A Cost-Effective, 2,048 Core InfiniBand Cluster at UTC for Campus Research and Education," to support a 2,048-core AMD-based HPC cluster. These resources are being deployed in FY2020.

Important technical advancements achieved in FY2019 include these highlights:

- Technical collaborations within SimCenter led to the creation of the "Digital Twins" swimlane that launched on July 1, 2019, and has already received its first NSF funding for engineering curriculum development.

† *Research in Undergraduate Institutions (RUI)*

- UTC's first virtual private cloud was procured and deployed with CEACSE support in the SimCenter to support High-Performance Computing and High-Throughput Computing
- UTC hosted a petascale computing workshop for approximately ten attendees. The workshop included instruction in MPI, Python, CUDA, software engineering best practices, and other core competencies in HPC.
- Dr. Francesca Leasi, as a result of a Faculty Initiation Award (details below), began a series of workshops called the Southeastern Computational School. The first annual workshop, hosted at UTC, brought in developers/instructors for the QIIME2 software, a microbiome bioinformatics platform used to solve a wide range of computational biology problems. The 25 attendees included faculty and students from 14 universities across the nation. The workshops will continue annually, with the aim of increasing educational opportunities and fostering new collaborations in computational biology.
- As a result of CEACSE funding, Dr. Azad Hossain convened the Inaugural Workshop of Southeastern Computational and Geospatial Environmental Hydrology, a multi-institutional group he founded with the help of Dr. Mustafa Altinakar at the University of Mississippi National Center for Computational Hydroscience and Engineering (NCCHE). The 28 attendees from UTC, NCCHE, and Tennessee Technological University found common ground in their research efforts and declared a shared vision for regional collaboration on federal funding opportunities and beyond. The next workshop will be held at NCCHE in FY2020.

Additionally, we began competitions for two new CEACSE programs: Faculty Initiation and Opportunity Awards, and Distinguished Lecture Series Grants. We awarded four Initiation/Opportunity Awards and four Lecture Series Grants in FY2019. Initiation Awards offer $15,000 (or up to $25,000 with 50% match on the additional funds from startup or other sources) to incoming faculty. This amount can, for example, provide a small amount of summer support, purchase necessary materials, cover conference travel, and allow the awardee to hire an hourly student assistant—all crucial pieces of kickstarting an assistant professor's career. The Opportunity Award portion of the competition allows established faculty to apply for a small amount of funding to help them pivot their research focus to something entirely new to them. The Distinguished Lecture Series program provides up to $2,500 (travel costs and a small honorarium) for a UTC faculty member to invite an accomplished researcher in their field to speak at UTC. All lectures are public, and promising research collaborations have resulted from each.

Dr. David Giles (above right), UTC Associate Professor, Biology, Geology and Environmental Science, and invited speaker Dr. Cranos Williams, Associate Professor, Electrical and Computer Engineering, North Carolina State University. Dr. Williams spoke to Dr. David Giles' class in Spring 2019. Dr. Williams was sponsored by a Distinguished Lecture Series grant received by Dr. Hong Qin.

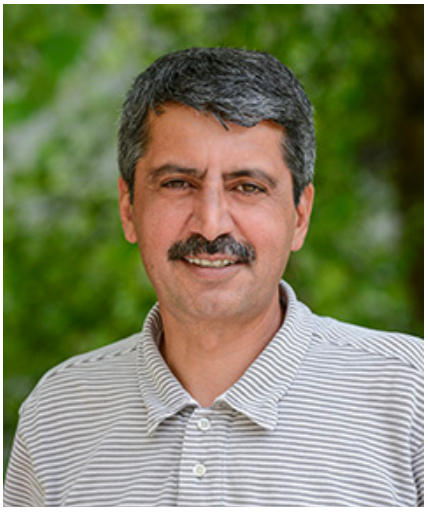
In collaboration, SimCenter and the Office of the Vice Chancellor for Research continue to foster a rapidly expanding and enhancing culture of securing external funding as an outcome of seed research funding provided by CEACSE. We recognize the challenges for faculty to excel in attracting extramural funding while meeting all aspects of meritorious scholarship. We provide support through the Office of Research and Sponsored Programs (ORSP) and our in-house Grant Administrator, through focus on opportunities that are designed to lead to larger funding awards, and through development of strategic partnerships. CEACSE is emerging as a nexus of research incubation, HPC and data science, and faculty resources that complement and supplement ORSP's offerings and add to those of faculty home departments.

NEW PRINCIPAL INVESTIGATORS ON EXTRAMURAL GRANT PROPOSALS

DR. ELENI PANAGIOTOU, first-year Assistant Professor in Mathematics at UTC in 2018-2019, served as PI on a grant proposal to the NSF Computational Mathematics program. The proposal, on topological modeling of polymer entanglement, was funded for $125,000. The project is a complex innovation in her area, with multifaceted applications. This funding is a signal accomplishment for Dr. Panagiotou, not least because she was successful in her first NSF proposal. Her co-PI, Dr. Jin Wang, is also mathematics faculty at UTC. This proposal was funded under the Research in Undergraduate Institutions (RUI) designation, which means it prioritizes undergraduate researcch eperiences, a prime goal of UTC.

DR. CRAIG TANIS, Assistant Professor in Computer Science at UTC, served as PI on a grant proposal to the NSF CyberTraining program (Training-based Workforce Development for Advanced Cyber-infrastructure). This proposal outlined a summer bootcamp and 9-month mentoring program designed to jumpstart introductory-level students' interest in HPC. These paired efforts include matching students with domain scientists from Oak Ridge National Lab. The result is increased engagement with HPC, from both the student and domain scientist perspectives: students hone their expertise and researchers expand their R&D capacity. Though the proposal was not funded, it activated Dr. Tanis; received favorable reviews; and fostered new collaborations with Tennessee Technological University (TTU), who have received two awards from this program in the past. Efforts to revise and resubmit are underway, with continued TTU collaboration.

DR. FARAH KANDAH, Associate Professor in Computer Science at UTC, served as PI on three grant proposals to NSF: Campus Cyberinfrastructure (CC*), Secure and Trustworthy Cyberspace Education (SaTC EDU), and Secure and Trustworthy Cyberspace Core (SaTC Core). The CC* proposal was funded for $499,663. This project will revolutionize networking capabilities for the entire UTC campus. The two SaTC proposals are still under review. The SaTC EDU project is a multi-institutional (Auburn University and Sonoma State University) collaboration to develop two undergraduate courses in cybersecurity-centric cloud computing. The SaTC Core proposal outlines a hardware-software codesign framework for cybersecurity, demonstrated in smart cities applications. The foundational work for this proposal is the core focus of the CPS swimlane for FY2020.

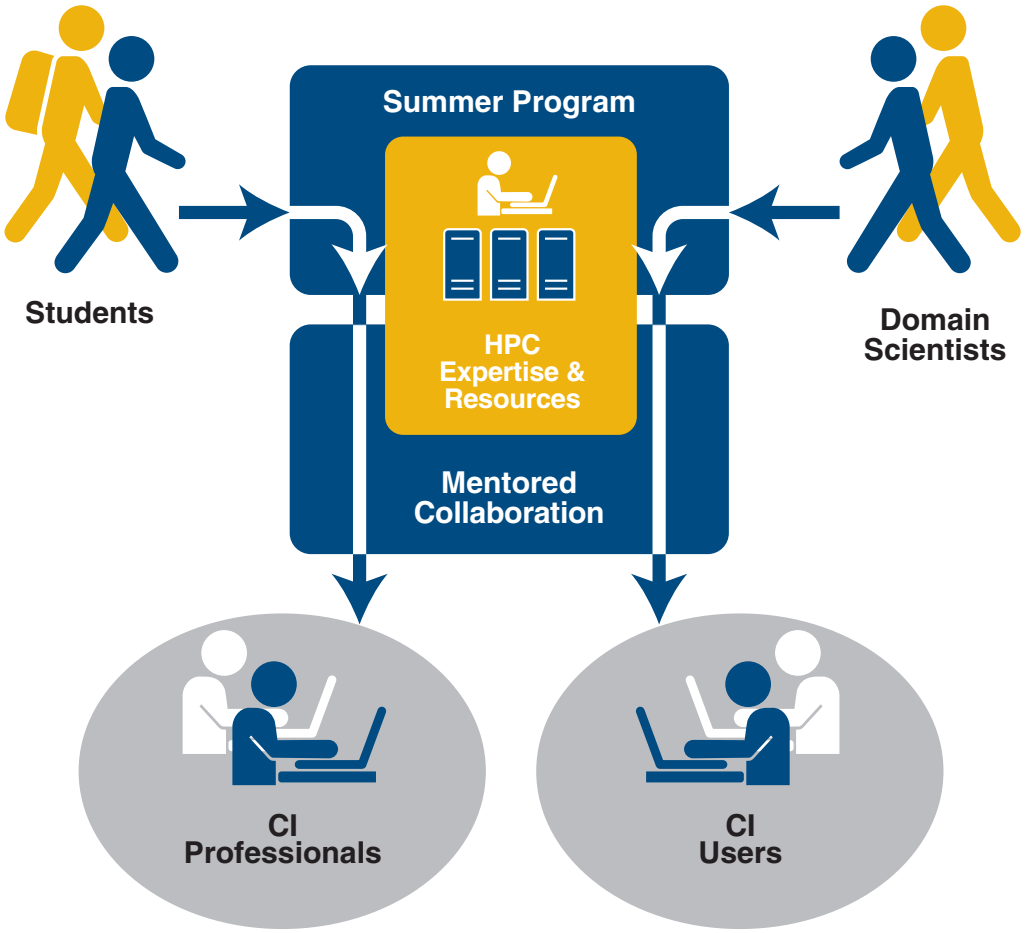


DR. ABDOLLAH (ABI) ARABSHAHI, SimCenter Research Professor at UTC, now serves as PI on an NSF grant awarded to former UTC Mathematics professor Dr. Feng Bao. The project, on modeling of stochastic differential equations, signals a leap forward for Dr. Arabshahi, who, in addition to being a first-time PI, is a first-time proposer to NSF. As a result of assuming the PI role of this award and serving as co-PI on a new NSF award for two UTC-led Digital Twin Workshops, Dr. Arabshahi is positioned to accelerate his proposal development efforts and bring in more research funding for his work with the SimCenter. This proposal also carries the RUI designation.

WORKFORCE DEVELOPMENT

Along with its recent research infrastructure improvements, SimCenter has established a new goal of pursuing workforce development initiatives. Tennessee has a critical need for skilled workers, especially in STEM and production fields. Chattanooga and Hamilton County in particular are replete with opportunities to support economic and personnel growth in these areas.

High-performance computing (HPC) is an increasingly central pillar of production development, given the expansion of Industry 4.0—a growing reliance on artificial intelligence, modeling and simulation, and other computationally oriented efforts—in manufacturing contexts. Preparing students to enter this new workforce is central to the SimCenter's efforts.



CyberTraining model for workforce development, from students and domain scientists to CI Professionals and Users.

SimCenter faculty have submitted two proposals toward this goal in FY2019. The first, an NSF CyberTraining grant, proposed a summer bootcamp and 9-month mentoring program designed to jumpstart introductory-level students' interest in HPC. These paired efforts include matching students with domain scientists from Oak Ridge National Lab. The result is increased engagement with HPC, from both the student and domain scientist perspectives: students hone their expertise and researchers expand their R&D capacity.

Though the proposal was not funded, it activated Dr. Craig Tanis, a faculty member who had previously not been active as a PI in grant proposals; received favorable reviews; and fostered new collaborations with Tennessee Technological University (TTU), who have received two awards from this program in the past. Efforts to revise and resubmit are underway, with continued TTU collaboration.

The second proposal born of the SimCenter's turn to workforce development and HPC was submitted to (and funded by) NSF's ECR: PEER program—Education and Human Resources Core Research: Production Engineering Education and Research. The interdisciplinary project responds to a call for innovative approaches to workforce development–oriented education in production engineering. With the acceleration of Industry 4.0 comes the need for integration with Education 4.0— specifically Engineering Education 4.0—to bring together cutting-edge educational technology and methods with advances in production engineering technology.

The project's goal is to bring together digital twin technology experts from both academia and industry to create a roadmap for production engineering education that includes significant exposure to strategic digital twin planning, development, and implementation. A secondary outcome will be a conception of an ideal digital twin knowledge worker, toward which the education plan will be oriented. This work will be accomplished through two 2-day workshops, one at each of UTC and TTU. The interdisciplinary proposal team includes Dr. Skjellum, Dr. Abi Arabshahi (SimCenter Research Professor), Dr. Jennifer Ellis (Education faculty), and Bailey Kirby (Grants Administrator, serving as research coordinator), marking significant progress in expanding and accelerating research collaborations across campus and the state. (See also pages 10-11.)

SELECTED FY2019 PUBLICATIONS AND PRESENTATIONS

C. Ratchford and **J. Wang**, "Multi-scale modeling of cholera dynamics in a spatially heterogeneous environment." Under review (for journal publication), 2019.

K. Yamazaki, C. Yang and **J. Wang**, "A partially diffusive cholera model based on a general second-order differential operator." Under review (for journal publication), 2019.

J. Yang, C. Modnak and **J. Wang**, "Dynamical analysis and optimal control simulation for an age-structured cholera model." Under review (for journal publication), 2019.

J. Bai, C. Yang, X. Wang and **J. Wang**, "Modeling the within-host dynamics of cholera: Bacterial-viral-immune interaction." Under review (for journal publication), 2019.

T. D. Loveless, B. Patel, **D. Reising**, R. Roca, M. Allen, L. W. Massengill, and D. McMorrow, "Single Event Transient Spectroscopy," *in review, IEEE Trans. Nucl. Sci.*, Jan 2020.

B. Patel, M. Joplin, R. C. Boggs, **D. R. Reising**, M. W. McCurdy, L. W. Massengill, and **T. D. Loveless**, "Ionizing Radiation Effects Spectroscopy for Analysis of Total-Ionizing Dose Degradation in RF Circuits," *IEEE Trans. Nucl. Sci.*, vol. 66, no. 1, pp. 61-68, Jan. 2019.

H. Qin, "Estimating network changes from lifespan measurements using a parsimonious gene network model of cellular aging." BMC Bioinformatics, tentatively accepted with minor revisions, 2019

Caleb Powell, Jacob Motley, **Hong Qin**, and **Joey Shaw**, "'Born digital,' a field-to-database solution for collections-based research using collNotes and collBook." Accepted by Botany, 2019.

S. Abbas, N. A. Arifi, M. Benchohra, and **J. R. Graef**, Random coupled systems of implicit Caputo-Hadamard fractional differential equations with multi-point boundary conditions in generalized Banach spaces, *Dynamic Systems and Applications*, 28 (2019), 329–350.

S. R. Grace, **J. R. Graef**, and E. Tunc, "On the boundedness of nonoscillatory solutions of certain fractional differential equations with positive and negative terms," *Applied Mathematics Letters* 97 (2019), 114–120.

J. R. Graef, S. R. Grace, and E. Tunc, "Oscillation criteria for even-order differential equations with unbounded neutral coefficients and distributed deviating arguments," *Functional Differential Equations* 25 (2018), 143–153.

J. R. Graef, S. R. Grace, and E. Tunc, "Oscillatory behavior of third order nonlinear differential equations with a nonlinear nonpositive neutral term," *Journal of Taibah University for Science* 13 (2019), 704–710.

J. R. Graef, S. Heidarkhani, **L. Kong**, and A. Salari, "Three weak solutions to a degenerate quasilinear elliptic system," *Le Matematiche*, LXXIV (2019), 191-210.

J. R. Graef, S. Ho, **L. Kong**, and M. Wang, "A fractional differential equation model for bike share systems," *Journal of Nonlinear Functional Analysis* 2019 (2019), Article ID 23, 14pp.

L. Kong, "A degenerate elliptic system with variable exponents," *Science China Mathematics*. 62 (2019), 1373–1390.

S. R. Grace and **J. R. Graef**, "Oscillatory behavior of second order nonlinear difference equations with a nonlinear nonpositive neutral term," *Miskolc Mathematical Notes*, to appear.

S. R. Grace, **J. R. Graef**, and E. Tunc, "On the asymptotic behavior of solutions of certain integro–differential equations," *Journal of Applied Analysis and Computation*, to appear.

J. R. Graef, S. R. Grace, and E. Tunc, "Asymptotic behavior of solutions of higher order fractional differential equations with a Caputo-type Hadamard derivative," *Progress in Fractional Differentiation and Applications*, to appear.

N. Prabaharan, C. Dharuman, **J. R. Graef**, and E. Thandapani, "New oscillation criteria for second order quasi-linear differential equations with a sub-linear neutral term," *Applied Mathematics E-Notes*, to appear.

S. Shokooh and **J. R. Graef**, "Existence and multiplicity results for non-homogeneous Neumann problems in Orlicz-Sobolev spaces," *Rendiconti del Circolo Matematico di Palermo Series* 2, to appear.

A. Da, B. Hazarika, **J. R. Graef**, and R. P. Agarwal, "Global attractivity of solution of functional nonlinear integral equations in two variables," submitted for publication.

A. Dogan and **J. R. Graef**, "Existence of positive solutions to multi-point third order problems with sign changing nonlinearities," submitted for publication.

S. R. Grace, **J. R. Graef**, I. Jadlovska, "Oscillatory behavior of second order nonlinear differential equations with mixed neutral terms," submitted for publication.

J. R. Graef, D. Beldjerd, and M. Remili, "Some new stability, boundedness, and square integrability conditions for third order neutral delay differential equations," submitted for publication.

J. R. Graef, D. Beldjerd, and M. Remili, "On stability, boundedness, and square integrability of solutions of certain third order neutral differential equations," submitted for publication.

J. R. Graef, S. R. Grace, and E. Tunc¸, "Oscillation of even-order nonlinear differential equations with sublinear and superlinear neutral terms," submitted for publication.

J. R. Graef, **L. Kong**, S. Heidarkhani, and S. Moradi, "Existence results for impulsive fractional differential equations with p-Laplacian via variational methods," submitted for publication.

J. R. Graef, **L. Kong**, **A. Ledoan**, and M. Wang, "Modeling online social network dynamics using fractional-order epidemiological models," submitted for publication.

J. R. Graef, O. Ozdemir, A. Kaymaz, and E. Tunc, "Oscillation of damped second order linear mixed neutral differential equations," submitted for publication.

J. R. Graef and B. Yang, "Positive solutions of the complementary Lidstone boundary value problem," submitted for publication.

A. M. Khatir, **J. R. Graef**, and M. Remili, "Stability, boundedness, and square integrability of solutions to third order neutral differential equations with delay," submitted for publication.

S. Padhi, **J. R. Graef**, and A. Kanaujiya, "Positive solutions to nonlinear elliptic equations depending on a parameter with Dirichlet boundary conditions," submitted for publication.

S. Abbas, N. A. Arifi, M. Benchohra, and **J. R. Graef**, "Periodic mild solutions of infinite delay evolution equations with non-instantaneous impulses," submitted for publication.

C. Gugg and **A. Ledoan**, "On a theorem of N. P. Romanoff," submitted for publication.

E. Eckels, S. Jin, **A. Ledoan**, and B. Tobin, "Lower bounds for the L1 norm of exponential sums," to be submitted.

S. Dhar and **L. Kong**, "Multiple anti-periodic solutions for a difference equation of higher order," submitted for publication.

S. Dhar and **L. Kong**, "Existence of multiple solutions for systems of fractional boundary value problems," to be submitted.

Davenport, M.E., Bonsall, M.B., & **Klug, H.** "Unconventional care: Offspring abandonment and filial cannibalism can function as forms of parental care." *Frontiers in Ecology & Evolution*. 7:1–11. 2019.

Klug, H. & Bonsall, M.B.B. "Filial cannibalism can facilitate the evolution of parental care." *Proceedings of the Royal Society B*. Provisionally accepted.

Bathi., J.R. and Roy., S. "Computer Tools for Urban Hydrology and Water Quality Management." S*ustainable Water: Resources, Management and Challenges*, Gude., V. G., Gadhamshetty, V. and Kandiah., R, editors. Sustainable Water: Resources, Management and Challenges, Nova Sciences Publishers, Inc. (Book chapter, submitted, review comments received on 8/9/2019).

Palchoudhury, S., Ramasamy, R., Gupta, R.K., Gupta, A., "Flexible supercapacitors: a materials perspective." Front Mater, 2019. 5:p. 83. Impact Factor: 2.69

Boutchuen, A., Zimmerman, D., Aich, N., Masud, A.M., **Arabshahi, A., Palchoudhury, S.**, "Increased plant growth with hematite nanoparticle fertilizer drop and determining nanoparticle uptake in plants using multimodal approach." *J Nanomater*, 2019. 2019:p. 6890572. Impact Factor: 2.23

Palchoudhury, S., Arabshahi, A., Gharge, U., Albattah, A., George, O., Foster, Y., "Integrated experimental and computational approach for nanoparticle flow analysis." *Phys Lett A*, 2019. 383:p. 1615. Impact Factor: 2.087

Gayen, B., **Palchoudhury, S.**, Chowdhury, J. "Carbon dots: a mystic star in the world of nanoscience." *J. Nanomater*, 2019 (accepted) Impact Factor: 2.23

Palchoudhury, S., Jungjohann, K., **Weerasena, L.**, **Arabshahi, A.**, Gharge, U., Albattah, A., Miller, J., Patel, K., Holler, R., "Enhanced legume root growth with pre-soaking in α-Fe2O3 nanoparticle fertilizer." *RSC Adv*, 2018. 8:p. 24075. Impact Factor: 3.049

Palchoudhury, S., *Strategic applications of measurement technologies and instrumentation*. (Book) IGI Global, 2018.

Gunasekera, S., Weerasena, L., **Saram, A.**, Oluwakorede, A. (2019). Exact inference for the Youden index to discriminate individuals using two-parameter exponentially distributed pooled samples. *Biostatistics & Epidemiology* 3(1),38-61, doi: 10.1080/24709360.2019.1587264

FUNDED PROPOSALS IN FY2019

In collaboration, the SimCenter, and the Office of the Vice Chancellor for Research foster a rapidly expanding and enhancing culture of securing external funding. 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) via an in-house Grant Administrator, through focus on opportunities that are designed to lead to larger funding awards, and through development of strategic partnerships. Our efforts drive three CEACSE funding competitions per year and encourage 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 FY2019, for a total of $2,623,106.

Title	PI	Funding Agency	Amount
RUI†: Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems	Dr. Abdollah Arabshahi	NSF	$42,269
RUI†: Computational Methods for Measuring Topological Entanglement in Polymers	Dr. Eleni Panagiotou	NSF	$125,000
CC* Networking Infrastructure: Advancing High-speed Networking at UTC for Research and Education	Dr. Farah Kandah	NSF	$499,663
CAREER: A probabilistic gene network model of cellular aging and its application on the conserved lifespan extension mechanisms of dietary restriction	Dr. Hong Qin	NSF	$137,136
REU Site: ICompBio - Engaging Undergraduates in Interdisciplinary Computing for Biological Research	Dr. Hong Qin	NSF	$351,108
Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education	Dr. Hong Qin	NSF	$549,888
CC* Compute: A Cost-Effective, 2,048 Core InfiniBand Cluster at UTC for Campus Research and Education	Dr. Tony Skjellum	NSF	$392,235
CICI: Data Provenance: Collaborative Research: Provenance Assurance Using Currency Primitives	Dr. Tony Skjellum	NSF	$34,866
Contract: Systems Software Performance and Optimization on Emerging Scalable Platforms	Dr. Tony Skjellum	Sandia National Laboratory	$49,999
RevV! - Data Analytics to Fast-Forward Product Development and Job Creation In Tennessee	Dr. Tony Skjellum	Oak Ridge National Laboratory	$250,000
SHF: Medium: Collaborative Research: Next-Generation Message Passing for Parallel Programming: Resiliency, Time-to-Solution, Performance-Portability, Scalability, and QoS	Dr. Tony Skjellum	NSF	$174,942
SHF: Small: Collaborative Research: Coupling Computation and Communication in FPGA-Enhanced Clouds and Clusters	Dr. Tony Skjellum	NSF	$16,000

Publications and Presentations (Cont.)

J. Cho, A. Alharin, Z. Hu, **N. Fell**, and **M. Sartipi**, "Predicting Post-stroke Hospital Discharge Disposition Using Interpretable Machine Learning Approach". Submitted to IEEE Big Data Conference 2019.

F. Kandah, **B. Huber**, **A. Altarawneh**, **S. Medury**, and **A. Skjellum**. "BLAST: Blockchain-based Trust Management in SmartCities and Connected Vehicles Setup." 2019 IEEE High Performance Extreme Computing Conference (HPEC'19), 2019.

F. Kandah, J. Cancelleri, **D. Reising**, **A. Altarawneh**, and **A. Skjellum**. "A Hardware-Software Codesign Approach to Identity, Trust, and Resilience for IoT/CPS at Scale." The 2019 IEEE International Conference on Internet of Things (iThings), 2019.

S. Schmitt, **F. Kandah**, and D. Brownell. "Intelligent threat hunting in software-defined networking." In 2019 IEEE International Conference on Consumer Electronics (ICCE), pages 1–5, Jan 2019.

F. Kandah, **B. Huber**, **A. Skjellum**, and **A. Altarawneh**. "A Blockchain-based Trust Management Approach for Connected Autonomous Vehicles in Smart Cities." In 2019 IEEE 9th Annual Computing and Communication Workshop and Conference (CCWC), pages 0544–0549, Jan 2019.

Michael K. Danquah, **Haobo Guo**, Kei Xian Tan, Manoo Bhakta. "Atomistic probing of aptameric binding of CD19 outer membrane domain reveals an "aptamer walking" mechanism." *Chemical Engineering Journal* (under review).

Caleb Acquah, Yi Wei Chan, Sharadwata Pan, Lau Sie Yon, Clarence M. Ongkudon, **Haobo Guo**, **Michael K. Danquah**. "Aptamer-anchored poly(EDMA-co-GMA) monolith for high throughput affinity binding." Scientific Report (under review).

Jaison Jeevanandam, Kei X. Tan, **Michael. K. Danquah**, **Haobo Guo**, Andrew Turgeson. "Advancing aptamers as molecular probes for cancer theranostic applications – the role of molecular dynamics simulation." Biotechnology Advances (under review).

† *Research in Undergraduate Institutions (RUI)*

RESEARCH ASSOCIATES

DR. RYAN MARSHALL is a postdoc in the SimCenter who works primarily for Dr. Skjellum. He received his MS in Computer Science and PhD in Engineering from Tennessee Tech. His main focus in FY2019 was to look for new ways to make HPC technologies (software in particular) accessible to researchers in other fields. Many are still using older software that cannot support the expanded capabilities of the modern HPC systems. While they may have some programming knowledge, these researchers are usually not experts in such technologies and need to bring in outside help. His goal is to reduce that need through collaboration by making tools that are user-friendly and able to be integrated into their workflows.

Currently Dr. Marshall is developing a learning algorithm for the multi-objective set covering problem with Dr. Lakmali Weerasena in the Math Department. Additionally, he is collaborating with various groups at LLNL, Auburn University, UAB, Tennessee Tech, and UC London to develop versions of MPI that are fault tolerant and/or 64-bit compatible.

Student mentoring is an important part of his work, including undergraduates who are intermediate programmers. He is planning to publish the results from his current projects and likely continue working with these groups to expand the scope of their work together.

MARTIN RUEFENACHT is a Term Researcher in the SimCenter. He received his MPhys in Computational Physics and MSc in Research Pervasive Parallelism from the University of Edinburgh, Scotland, UK. He is currently working on his PhD in Pervasive Parallelism at the University of Edinburgh.

Martin's projects in FY2019 centered on ExaMPI, the MPI implementation he and his collaborators (including Dr. Skjellum) are writing. They are developing a research MPI implementation instead of a production library, which will hopefully yield greater research output from the community when it is more stable by allowing them to modify a lean library instead of behemoths. All his other work is based on ExaMPI, fault tolerance, and user-level schedules.

In addition to ExaMPI, he is working on the LemonSpotter project, along with Carson Woods, a UTC Computer Science and Engineering undergraduate student. (See page 20.) It is a test generation framework specific to MPI (for the moment). The goal is to generate a huge number of tests and be able to test the MPI implementations thoroughly compared to hand–written test suites. He is also working on language interface related issues for MPI, including new language interfaces and integrating Python tools into an MPI application. A continual side project is writing papers toward further development of the MPI standard.

His work also continued an existing research collaboration on fault tolerance with Dr. Ignacio Laguna from LLNL and spawned a new collaboration with Sandia National Labs on partitioned collectives. Martin spent three weeks at Sandia as part of these efforts. Other research collaborations are continuing with Dr. Puri Bangalore at UAB and Dr. Daniel Holmes in Edinburgh.

Martin will be leaving the SimCenter at the end of September 2019 but will continue to work with Dr. Skjellum, University of Edinburgh, Sandia, Boston University, and Livermore for many more years.

STUDENT PROFILES

JAMES TRIMBLE is a Computational Science PhD student with a concentration in Computational Engineering. Currently a Major in the Air Force, James graduated from the Air Force Academy in 2006 with a degree in electrical engineering. He was later accepted to the faculty pipeline program, which means he will return to the Air Force Academy as an instructor in the future. That program led him to UTC to study under his advisor, Dr. Pack, who was one of his instructors during his undergraduate time at the Air Force Academy.

James works in the Unmanned Systems Lab on the first floor of the SimCenter. He has been involved with several projects: (1) The malaria project uses UAVs to map an area, identify potential mosquito larvae sites, and deliver an environmentally safe larvicide. (2) Another project involves developing a system for a swarm of UAVs to search, find, and locate electromagnetic sources like radar sites, two-way radios, beacons, etc. (3) Researchers use an EKG helmet to monitor brainwaves, which they process and use to determine user input for controlling multiple UAVs.

James's research is on network connectivity for unmanned aerial vehicles, focusing on arranging the agents in the system in a way that achieves desired levels of connectivity at different points throughout a UAV team's mission. For his dissertation, James uses the MATLAB Distributed Computing Server on Qbert, one of the cluster computers in the SimCenter. He often has to run many simulations with different parameters so he can compare different methods or show how his contributions have made an improvement. Using the parallel processing capabilities on QBert speeds up the time required to run these simulations.

James hopes to graduate this summer and return to the Air Force Academy, but the Unmanned Systems Lab will continue to develop current projects he's involved in.

JHIIN JOO earned her Bachelor's degree in Electrical Engineering and Computer Science from the Kyungpook National University, and her Master's degree in Electrical Engineering from the University of Southern California. She received her PhD in Computational Engineering from UTC in August 2019.

Her research, under Dr. Kidambi Sreenivas and Dr. James Newman, is to capture and analyze the turbulent wall-pressure fluctuations. She uses large-eddy simulation for the large scale motions of turbulence and a wall-adapting local eddy-viscosity model for the smaller-scale motions. Her work uses the finite-element method formulation with the streamwise/upwind Petrove-Galerkin method as the numerical methods to solve the governing equations.

The proposed inflow generation method was implemented and validated for generating the inflow turbulent velocity profile at the inlet of the computational domain to maintain the turbulent characteristics throughout the simulation. Non-reflection boundary conditions were imposed at the top and exit of the domain to prevent contamination of the numerical results.

Jhiin plans to continue this area of turbulence modeling after graduation, either in academia or industry.

STUDENT PROFILES


Photo by Janet Fang

CARSON WOODS is a rising senior pursuing his BS in Computer Science: Data Science and Mathematics (double major). He is actively doing research on two separate projects, one for Dr. Tony Skjellum and the second for Dr. Li Yang.

This summer, he was a research and development intern at Sandia National Labs in Albuquerque, New Mexico. He worked on building scalable systems software for high-performance supercomputers. Specifically, he worked on building a portable computing environment that other researchers could easily install to reproduce experiments to validate results or simply have a stable research environment that runs at high performance on next-generation hardware.

His primary research focus for the previous year was in high-performance computing, high-performance machine learning, and cybersecurity education. With Dr. Skjellum, he researched how low-precision linear algebra can reduce the time it takes to train a neural network without sacrificing the neural network's accuracy. After finishing that project, they started a new project to develop a testing tool to examine MPI implementations for performance and compliance to the MPI standard. Additionally, with Dr. Li Yang, he has been developing tools that professors and students can use to improve how cybersecurity topics are taught in classrooms.

Carson plans to continue to do research at the SimCenter with Dr. Skjellum. He also will be leading UTC's MocSec cybersecurity defense team and studying abroad in Tokyo, Japan, next spring and summer. Post-graduation his current plans include pursuing a graduate degree, ideally a PhD in Computer Science.

AARON CRAWFORD is a rising senior completing his Bachelor of Mechanical Engineering at UTC. He works with Dr. Kidambi Sreenivas, faculty in Mechanical Engineering.

In summer 2019, Aaron interned with the U.S. Army Aviation Development Directorate (ADD) stationed at NASA Ames. This group specializes in computational fluid dynamics and aeromechanics for rotorcraft. His internship project related to the Workshop for Integrated Propeller Prediction (WIPP) facilitated through the American Institute of Aeronautics and Astronautics (AIAA). The summer included a trip to attend this workshop at the recent AIAA Aviation Conference. While interning, he used the high-fidelity flow solver developed at Ames, called Helios, in conjunction with DOD High-Performance Computing resources to complete this research.

During the school year, he worked on this same project in-house using the software and CFD solver found at the SimCenter. Additionally, he participated in a project on CFD analysis for lower Manhattan. This project incorporated aspects of GIS as well as CFD.

After graduation, he plans to pursue a PhD in Mechanical or Aerospace Engineering, most likely with a concentration in thermo-fluids and CFD.

ALUMNI PROFILES

DR. DAVID COLLAO

graduated from UTC with an MS (2011) and PhD (2017) 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?

The focus of my PhD research was studying, via computational fluid dynamics simulations, how the operating stability of axial transonic compression systems was affected using a passive stability-enhancing method. The biggest challenge in this work was finding the right solver and grid parameters so that the simulation results resembled closely the available experimental results. For my MS thesis, I developed a piece of code that created a dataset called "spacing field" that computed optimal point spacing in 2D meshes based on solutions or just on mesh information. I also created a library of tools to manipulate that data.

How did the SimCenter factor into your work?

The SimCenter was involved in every single factor in my work. For my PhD work, I had a choice between two clusters (Big Frog and Papertape) on which to run my simulations, and I had the expertise of Dr. Webster, Dr. Sreenivas, and Dr. Arabshahi whenever I ran into problems with the solver or the mesh. While working on my master's degree, I had the guidance of Dr. Karman and worked with two other students doing related work.

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

I'm a software and algorithms engineer at Branch Technology. We develop software tools and use them to create 3D grids that are "printed" by robots via extrusion. The skills that are the most valuable in my current position are skills that I learned at the SimCenter: mesh generation, computational geometry, and software development for scientific computing.

Do you have any advice for current students?

Be willing to submit to the guidance of your professors. I found they're willing to share their knowledge. Also, enjoy your friends in grad school. The friendships I've made in grad school have been tightest and most lasting even though these friends are thousands of miles away. And have fun!

DR. PHILIP FACKLER

graduated from UTC with an MS (2013) and PhD (2017) 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 focus was mesh generation—more specifically, populating and smoothing point distributions to match an arbitrary spacing field (which actually doesn't involve a mesh). The part I'm most proud of was the dynamic population control. The algorithm could add and remove points as necessary to appropriately cluster points throughout the domain. From a single seed point, it could recursively spawn new points until the whole domain was filled in such a way that matched the spacing field pretty well and didn't require much smoothing.

How did the SimCenter factor into your work?

My experience at the SimCenter was relevant to practically all the work I did in my previous job at Branch Technology. I used data structures for working with structured and unstructured grids, searching and smoothing algorithms, spatial subdivision trees, etc.

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

I'm currently a Research Software Engineer at the Oak Ridge National Laboratory. The SimCenter provided education in computational simulation, mesh generation, parallelism with MPI and OpenMP, and numerical analysis. All of these things were discussed directly in the interview process, which led directly to me getting this position.

Do you have any advice for current students?

First, aim to write "good" code. There's a lot on the internet about that topic, but basically you're codifying knowledge, and you want that to be understandable to other people.

Second, get familiar with some of the tools that surround software development besides just programming languages. For example: version control (Git), build system (CMake, meson), package manager (conan, conda, CPack), testing (CTest, Boost.Test, catch2), documentation (doxygen), and continuous integration (jenkins, docker). These kinds of tools (and others, like IDEs, issue-tracking, and project management) are a big part of any software job, and you don't want to have to learn everything from scratch after you get started.

INDUSTRY COLLABORATIONS

International Maritime Security Associates, Inc. (IMSA)

This year, SimCenter began collaborations with International Maritime Security Associates, Inc. (IMSA), a small, veteran-owned business with operations centers in South Florida, Chattanooga, and London, UK. IMSA's primary goal is improved maritime operations through better information and intelligence. Central services include real-time risk management and overall cybersecurity, all integrated with existing response protocols. Their main product, the ARMS (Automated Risk Management Solution) Software Platform, puts real-time, location-specific risk and threat information at mariners' fingertips via a tablet-based dashboard interface.

SimCenter Director Skjellum collaborated with IMSA on a recently funded grant opportunity called RevV!, part of a $2.5 million manufacturing innovation program created by the State of Tennessee in partnership with the University of Tennessee and Oak Ridge National Lab (ORNL). The RevV program allows the winning manufacturers, product developers, and researchers access to state-of-the-art computing and other facilities at ORNL, in addition to up to $250,000 in funding.

The goal of this collaboration is for SimCenter personnel, including Dr. Skjellum and his students, to assist IMSA in accelerating their ability to pull, organize, and process large datasets. The high-performance computing resources and expertise of the SimCenter, paired with those at ORNL, will allow IMSA to complement their existing data-gathering infrastructure: their Global Intelligence, Information and Communications Center (G-I2C) maintains a carefully maintained source of information and intelligence available 24/7 to support mariners anywhere in the world.

Additionally, IMSA recently applied for a Small Business Innovation Research (SBIR) grant through the National Science Foundation (NSF). This award would allow IMSA to utilize SimCenter expertise to determine the feasibility of developing and using machine learning algorithms to predict any number of rapidly changing factors at sea, such as port delays.

Branch Technology

Branch Technology, a large-scale 3D printing company based in Chattanooga whose software team is led by UTC Computational Engineering PhD graduate Bruce Hilbert, is another recent SimCenter partner. Several SimCenter graduates and former employees have gone on to work for Branch, drawn in part by the company's distinction as the home of the world's largest freeform 3D printers. Branch's unique printing process creates cell-like lattices that mimic complex natural structures and have numerous applications, especially in construction. Dr. Hilbert and his team are employing techniques researched and invented at the SimCenter to develop their processes.

SimCenter collaborations with Branch include placing a Computational Science PhD student, Sai Medury, in a 6-month internship supported via a supplement to an NSF grant helmed by Dr. Tony Skjellum. Sai will tackle significant problems Branch's engineers have lacked the bandwidth to address, further accelerating the company's growth and development. He has already contributed significantly to their codebase.

Branch and SimCenter have begun exploring joint funding opportunities; preparing additional internships; determining how to further collaborate on workforce development of future engineering workforce in additive manufacturing; and exploring digital twin technologies and their implications for research, education, and additive manufacturing in industry.

SIMCENTER STAFF

Left to right: Holley Beeland, Bailey Kirby, Kim Sapp, Dr. Ethan Hereth, Anna Lane, and Dr. Tony Skjellum

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 BFA in Art from Mississippi State University in 1988. As 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 graphics and web presence for the Graduate School, the Office of the Vice Chancellor for Research, URaCE, the SimCenter, Computational Science PhD Program, Center for Informatics & Progress (CUIP), Interdisciplinary Geospatial Technology Lab (IGTLab), and CEACSE.

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 BS and MS from the University of Central Arkansas in 2005 and 2007, respectively, and received his PhD 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.

BAILEY KIRBY 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 BA in English from Texas A&M University in 2013 and her MA in Technical Communication from Texas Tech University in 2017.

ANNA LANE is the Accounting Coordinator for the Vice Chancellor for Research & Dean of the Graduate School also providing support for CUIP, the Computational Science PhD Program, the IGTLab, and the SimCenter. Prior to joining the SimCenter in 2018, 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 providing support for CUIP, the Computational Science PhD Program, IGTLab, and the SimCenter. 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 Multidisciplinary Research Building.

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