SimCenter

Center of Excellence in Applied
Computational Science and Engineering

2020-2021 ANNUAL REVIEW

THE UNIVERSITY OF TENNESSEE
CHATTANOOGA

CONTENTS

PUBLICATION RESOURCES

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MESSAGE FROM THE DIRECTOR

Welcome to the SimCenter Annual Report for Fiscal Year 2021 (July 1, 2020–June 30, 2021). 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.

The SimCenter, the Center of Excellence in Applied Computational Science and Engineering, is UTC's Research Accelerator and Research Computing Core Facility. The 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 program at UTC, the 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, the 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, Chemical Engineering are represented here.

During FY2021, we revamped and enhanced our existing research thrusts to include eight specific areas: Advanced Modeling and Simulation, Critical Infrastructure Protection, Cybersecurity and Cyber-physical Systems, Digital Twins, Environment, Extreme Systems, Health and Biosystems, and High-Performance Computing and Algorithms. Critical Infrastructure Protection is the newest, formed just before the end of the fiscal year. It subsumed the Energy thrust, focusing more on the

security aspects of that area. We will spend FY2022 activating faculty in relevant research areas, seeking funding for concentrated research and education efforts, and accelerating workforce development in this crucial and expanding piece of national defense.

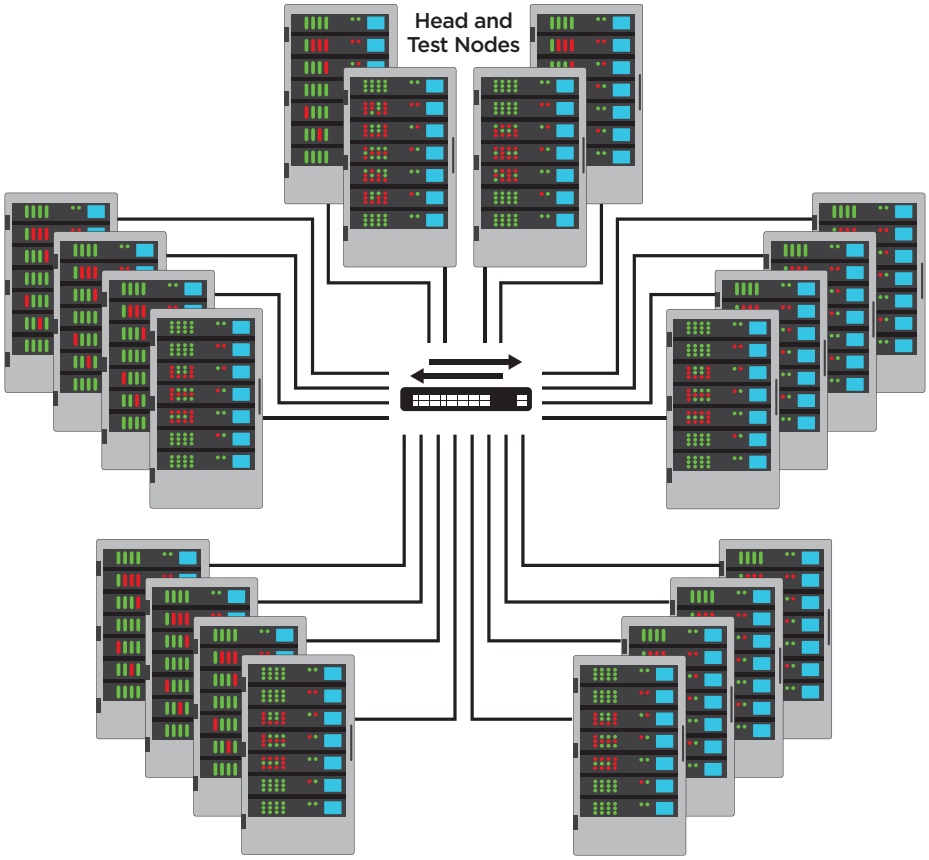
The SimCenter's goal is also to move beyond UTC and engage new participants from the community, state, and region. We look forward to an ever-expanding portfolio of R&D centered on modeling and simulation, high-performance computing, and advanced algorithms in our swimlane areas and beyond.

Sincerely,

DR. ANTHONY (TONY) SKJELLUM *has been the Director of the SimCenter since August 2017. He received his 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 INFRASTRUCTURE

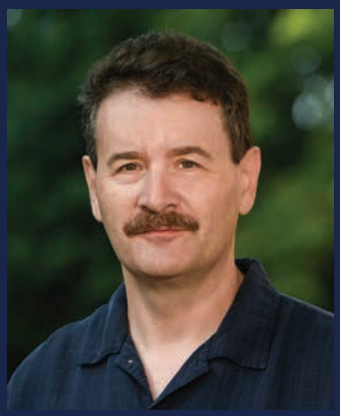
The Cyberinfrastructure at UTC SimCenter continues to improve. In this fiscal year, our NSF CC* Compute-funded cluster based on AMD EPYC2 processors reached full operation. A total of 2,560 x86-64 superscalar cores are supported with 100Gbit/s EDR InfiniBand networking. The system itself connects to the new research network also supported by NSF under an effort led by Dr. Farah Kandah. Our cluster is connected directly to this network at 100Gbit/s data transfer rates. Among other enhancements made to this cluster, a second high-performance network for experimentation has been added. Also, to work on next-generation AI workloads, the first two NVIDIA A100 Ampere GPUs were acquired, and put into early experimental use. Some of our users have already obtained significant performance gains in their applications through early experiments with the A100s.



A follow-on proposal in FY2022 is planned to NSF to ask for a complete complement of A100 GPUs to power the cluster for much greater machine-learning-workload performance (10x or more), and nearly a factor of four more performance for traditional high-performance computing workloads that emphasize double precision.

The research network extends to eight campus buildings, and provides, through Gigabit/s connectivity added by UTC Central IT, a minimum of 1 Gigabit/s access to every professor and laboratory desktop in these key academic buildings. High-performance access off-campus and inter-campus is also possible for specialized research applications. Access to the systems remains free for all professors and postdocs, and also undergrads and grad students mentored by advisors on campus.

Our NSF-funded Planning grant for advanced cyberinfrastructure collaboration and sharing, together with MTSU and TnTech, started, albeit a bit slowly due to COVID-19 restrictions. In FY2022, joint seminars, meetings, and collaborative efforts related to advanced cyberinfrastructure will be commenced with our partner universities in pursuit of better cyberinfrastructure and networking (human and computer) across middle Tennessee.



DR. MIKE WARD received his BS in Computer Science from Michigan Technological University, his MS in Computer Science from UTC, and his EdD in Education from UTK. As the Cyber Infrastructure Facilitator at the SimCenter, Dr. Ward helps implement and maintain the HPC infrastructure including the related hardware and software. He also assists faculty and students in understanding and using that infrastructure. Finally, as a former Network Security Analyst and System Administrator with UTC's central IT, he provides a knowledgeable conduit for topics such as cybersecurity and virtualization between the SimCenter and the rest of UTC. Significantly, he designed and implemented the first UTC Cybersecurity Lab and was instrumental in the 2019 modernization of the UTC Central IT compute infrastructure. In addition to his regular duties, he serves as an adjunct instructor at UTC, teaching Computer Science courses such as operating systems, networking, and cybersecurity, as well as some education courses.

COMMITMENT TO BROADENING PARTICIPATION IN COMPUTING

In 2017, the National Science Foundation (NSF) launched a new diversification initiative called Broadening Participation in Computing (BPC) in the Directorate for Computer and Information Science and Engineering (CISE). The goal of the initiative is to increase participation of underrepresented groups in computing disciplines: Black, Hispanic, American Indian, Alaskan Native, Hawaiian Native, and Native Pacific Islander individuals; all disabled individuals; all individuals from socioeconomically disadvantaged backgrounds; and all women. NSF encourages Principal Investigators to intentionally establish outreach activities and recruitment pipelines that target these groups.

The SimCenter recognizes the significance of these efforts and is working to align our recruitment, retention, and outreach practices with CISE goals. As we work to develop both center-level and individual PI BPC plans, we are improving ongoing efforts to involve students from underrepresented groups in computing degree programs and hands-on research.

In FY2021, the following students from underrepresented groups were among those employed by the SimCenter. We will continue to support these students, and those who come after them, in ways that specifically attend to the systemic barriers to their continued enrollment at UTC and their later success in the workforce—including but not limited to racism, sexism, and ableism.

- Clara Alsobrooks, BS Computer Science & Engineering
- Kasturi Barkataki, PhD Computational Mathematics
- Jamie Bowers, MS Mechanical Engineering
- Savannah Camp, MS Computer Science & Engineering
- Carmen Harvey, BS Civil Engineering
- Dallas Jones, BS Mechanical Engineering
- Akua Maame Korsah, MS Computational Mathematics
- Evelyn Namugwanya, MS Computer Science & Engineering
- Grace Nansamba, MS Computer Science & Engineering (PhD beginning Spring 2021)

Further recruitment and support sources will include the several ongoing NSF-funded Research Experiences for Undergraduates (REU) projects at UTC, the SimCenter-hosted Middle Tennessee Cyberinfrastructure Alignment Consortium (MTCAC) funded by the NSF Campus Cyberinfrastructure (CC*) program, and the UTC Undergraduate Research and Creative Endeavors (URaCE) Office.

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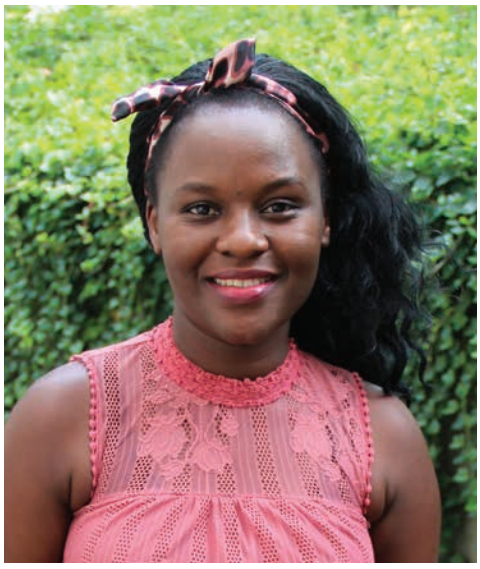


Evelyn Namugwanya, PhD Computer Science & Engineering

Grace Nansamba, PhD Computer Science & Engineering

SIMCENTER MISSION & VISION

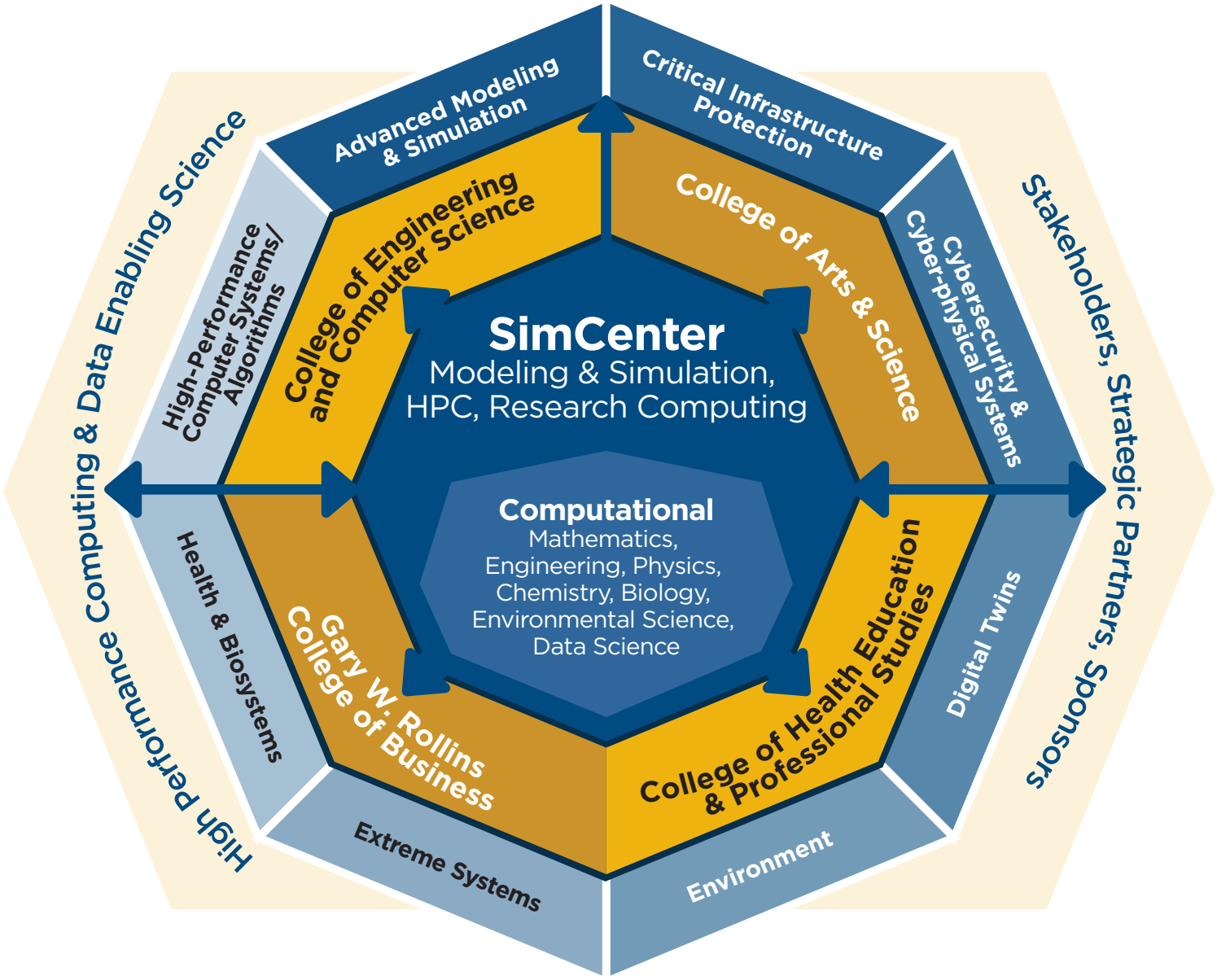
MISSION To establish, expand, and sustain a cohesive multidisciplinary effort in applied computational sciences through mentoring of students and faculty, seed funding in key thrust areas, and state-of-the-art research computing facilities.

VISION SimCenter makes impacts across UTC to help generate sustained growth in faculty research funding, excellence in integrated education and research, and growth in the number of Ph.D. graduates in these applied areas. We investigate, design, and deliver solutions to problems of importance to society in advanced modeling and simulation, high-performance computing, and data sciences. We train undergraduate and graduate students at UTC to become knowledge workers who help drive economic growth both locally and nationally. Our cohesive multidisciplinary efforts in applied computational sciences are recognized for their contributions to the community, the state of Tennessee, the region, and the nation.

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. FY2021 marked the 15th 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 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.

Some notable outcomes

- From CEACSE funds, we awarded eight core awards ($100,000) and one Initiation/Opportunity Award ($15,000) in FY2021.
- We launched one new research thrust: Critical Infrastructure Protection (led by Dr. Don Reising).
- Dr. Andrew Bailey has developed new collaborations with Thrive Regional Partnership, The Trust for Public Land, Lula Lake, SORBA Chattanooga, Southeastern Climbers Coalition, Land Trust for TN, TN River Gorge Trust, Southeastern Conservation Corps, and WaterWays.
- Dr. Eleni Panagiotou submitted an NSF CAREER proposal related to her CEACSE project. It has been recommended for funding.
- Dr. Sungwoo Yang received a Ruth S. Holmberg grant for his work. He also submitted a proposal to the NSF Engineering Research Initiative program.
- Dr. Abi Arabshahi submitted proposals to IBM on COVID-19 pulmonary airflow modeling and to the UT Biomedical Research Initiation Collaborative Grant program. Both were funded.
- Dr. Reetesh Ranjan submitted proposals to NASA ULI, the DEPSCoR Research Collaboration program, and the ORAU Ralph E. Power Junior Faculty Enhancement Awards program.
- Dr. Reetesh Ranjan and his students created AVF-LESLIE, a fully compressible multi-species reacting flow solver, and UTCFOAM, an in-house and extended version of OpenFOAM.

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), 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 a key provider of faculty resources that complement and supplement ORSP's offerings and add to those of faculty home departments.

FY2021 awardees

- Fernando Alda and Yu Liang: "Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome"
- David Giles, Steven Symes, and Bradley Harris: "From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes"
- Hamdy Ibrahim and Mohammad Mahtabi: "Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants"
- Daniel Loveless and Don Reising: "Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)"
- Mohammad Mahtabi and Hamdy Ibrahim: "Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials"
- Ashley Manning-Berg and Abi Arabshahi: "Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record"
- Hong Qin, Ziwei Ma, and Azad Hossain: "Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2"
- Reetesh Ranjan: "Modeling of Transition to Turbulence in Large Eddy Simulation using the Two Level Simulation Approach"

FIRST-TIME CEACSE AWARDEES

DR. YUNYE SHI joined the Department of Mechanical Engineering at UTC in August 2020. Before joining UTC, she was an Assistant Professor at St. Ambrose University in Iowa. She received her PhD from the University of Iowa (2016), and MSc and BSc from the Huazhong University of Science and Technology in China. She teaches courses in thermal-fluid sciences and conduct research in the area of biomass conversion technologies, biorenewable energy utilization, and techno-economic analysis of energy systems.

Biomass gasification is a series of complex processes that is highly nonlinear. Predicting the output of such processes is very important for system design and operation monitoring. Her CEACSE Faculty Initiation project aims to predict the output of gasification processes via machine learning approaches. A database is built with over 16,000 data collected from different gasification conditions. Biomass feedstock properties and operating parameters such as equivalence ratio, steam to air ratio, temperatures from various bed locations are selected as model features. Various machine learning models are trained and k-folds cross validation are used to determine the hyperparameters of the models. The models are then tested against the experimental data for accuracy evaluation. Among the models, random forest outperform all others and achieved high accuracy in predicting syngas composition and lower heating value of the syngas. The variable importance analysis shows that steam temperature, combustion zone temperature and equivalence ratios as the three most important features for the model. The next step of the work is to apply the developed models to biomass preprocessing processes such as carbonization. Carbonization is similar to gasification in that both processes are highly nonlinear, so hidden relationships between variables are sometimes hard to define in physical models. Using machine learning tools will open new opportunities for modeling and prediction.

DR. OSAMA OSMAN is the Assistant Professor of Intelligent Transportation Systems and Data Analytics in the Department of Civil and Chemical Engineering at UTC. He is also the Mobility Thrust Lead in the Center for Urban Informatics and Progress and the Founding Director of SMITS Lab at UTC.

His research focuses on mathematical and simulation modeling and analysis of connected vehicle and connected autonomous vehicle environments, application of advanced modeling and data analytics techniques for traffic control and congestion management, developing machine learning and deep learning algorithms for detection and prediction of risky driving behavior, and investigation of impact of emerging vehicular technologies and smart mobility on mobility, energy, and behavioral safety.

Dr. Osman's CEACSE project aims to develop an integrated simulation platform to enable studying interactions between heterogeneous road users (drivers vs. pedestrians, or car occupants vs. non-occupants). The integrated platform will allow collection and visualization of data about those interactions. To achieve this goal, the following objectives are being pursued:

- Develop an integrated simulator for heterogeneous road users that capitalizes on VR technology.
- Enable comprehensive behavioral data collection and visualization.
- Study drivers and pedestrians' behavior based on their interactions in roadway environments.

Currently, the team is working with the driving simulator to develop scenarios that can help develop the integration of a pedestrian in the loop. Next steps include acquiring a Head Mount Display to be integrated with the driving simulator as an important step before performing pilot experiments on the integrated platform.

DR. SUNGWOO YANG, an assistant professor, joined the Civil and Chemical Engineering Department at UTC in the Fall of 2017. He received his PhD at Duke University, then joined MIT as a postdoctoral fellow to conduct research within the Device Research Laboratory (with Prof. Evelyn Wang). Later, he became a research scientist at MIT in 2014. The focus of his research is on porous materials which intersect the multidisciplinary fields of solar energy harvesting and thermal energy storage. He aims to bring about transformational efficiency enhancements in energy conversion and storage, buildings, water, and transportation by manipulating optical, thermal, and adsorptive properties of porous materials with device level considerations. The focus of his research efforts will be directed towards both (1) fundamental research on developing new classes of hybrid materials for efficient energy conversions and storages, and (2) applied research on devices and systems including for full spectrum solar energy conversion, thermal energy storage, water harvesting, and energy efficient buildings.

Due to COVID-19, his project was not completed in FY2021 and will carry over into FY2022. His project involved the following activities in FY2021:

- The group finalized a synthetic method of OTTI aerogel that demonstrated high transmittance (95% solar-weighted).
- They synthesized ambiently dried aerogel that demonstrated ~ 90% transmittance that is equivalent to the best literature value.
- They are in the process of developing optical and thermal computational modeling using RTE and Mie theory.
- They built a lab-scale solar receiver.

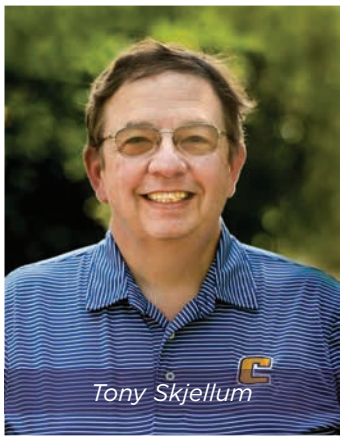
Outcomes include winning the Ruth S. Holmberg Grant, submitting an NSF-ERI proposal, beginning a peer-reviewed publication on ambiently-dried aerogels, and delivering an oral presentation at the Solar Energy Systems Conference. Anticipated next steps for the project / after the period of performance.

DR. ANDREW BAILEY teaches outdoor recreation, education and tourism in the Department of Health and Human Performance. He received his PhD in Education from the University of Minnesota, specializing in the use of outdoor activities and natural spaces to support human thriving. His research investigates the mutual benefits of the human/nature relationship, including economic impacts of outdoor recreation and tourism, as well as the psycho-physical benefits of exposure to natural environments. His CEACSE research project combined all of those research interests to investigate the true positive value of outdoor assets in the Chattanooga region.

Outdoor recreation is a central part of Chattanooga's identity. Visitors travel from across the globe to run the local rivers and test their climbing skills on the crags, while residents can enjoy routine outings in their own backyard. These protected spaces drive our tourism economy and enhance mental and physical health, but grasping the scale of the direct and indirect impacts has been an elusive endeavor. This project brought together experts in recreation and tourism, conservation, and public health to establish a baseline and trajectory of outdoor impacts in 16 counties surrounding the city of Chattanooga. Utilizing large-scale cellular tracking data, visitation and tourism impacts to 168 green spaces in the region were estimated. Preventive health care costs associated with park acreage were also included in the model, as well as preventive environmental mitigation costs associated with undeveloped land in the region. Machine learning was then applied to geospatial data to determine trends based on carrying capacity, biodiversity, climate change, and land development in the region. Of the $2.6 billion annually attributable to outdoor assets, the region could experience annual declines of $260 million in tourism and $30 million in environmental mitigation if current trends hold. These data will be used to support regional planning that promotes strategic, sustainable development that enhances public health and the regional economy, while protecting the natural treasures that make the area unique. Highly valuable and highly vulnerable areas will receive heightened attention through regional partnerships and funding strategies to ensure that residents of and visitors to the Chattanooga region can enjoy unspoiled natural beauty for years to come.

UPCOMING THRUST PROJECTS

Cyber Poverty



In cybersecurity, the "cyber poverty line" refers to a financial and technological situation where small businesses, individuals, and groups are unable to afford the cybersecurity they need in order to safely operate their systems, devices, and processes safely. Most devices now have some way of connecting to the internet, and a plethora of endemic and emerging threats—ransomware, computer viruses and worms, spyware, keyloggers, data extrusions, fake system updates, and botnets—plague large enterprises, home systems, and small businesses alike. But, the cost to maintain up-to-date and sufficient defenses and processes to thwart attacks and loss of time, money, data, use of the systems, and privacy is beyond large portions of society, both here in the United States and abroad. With recent efforts to increase internet access, support equity of access, and the importance of the internet for remote instruction during the COVID-19 pandemic, the acuity of lack of good security is ramping in its importance, with associated downsides of attack growing in their potential impact on the most vulnerable of consumers and businesses.

To combat such complex and evolving threats, Internet Service Providers (ISPs) generally do little to help consumers of their internet service beyond providing online help information and free antivirus software. This is the national norm. They do not monitor content or sources or destinations of data, and they rarely inform home and small office users about forensic information indicative of system takeover and the like. While managed models for remote installations are offered by ISPs for businesses, this solution may not be affordable within the construct of the cyber poverty line.

A better approach to the interactions of ISPs, consumers, and small-to-medium enterprises is possible that is affordable, provides for a collaborative relationship between the ISP and consumer, and offers an opportunity to price that management service equitably as it achieves its dual commercial and community service missions. Consumer privacy will be maintained, and many classes of threats to the operation of systems by end-users and small-to-medium enterprises can be thwarted while offering ISPs market differentiation and potential new income streams above and beyond "smart installation" and "smart network operations."

The use of added-value software in the router, modem, and, where appropriate, other devices supplied by an ISP can be coupled with blockchain technology, machine learning, and common device vetting to create a "safer space" to operate without as many threats or as obvious threats simply overrunning users of the Internet. This infrastructure architecture and associated prototyping is ongoing research at the SimCenter in the Cybersecurity and Cyber-physical Systems thrust, led by Dr. Farah Kandah.

XiveNet

In collaboration with researchers from Tennessee Technological University, Auburn University, and Oak Ridge National Laboratory, Drs. Skjellum and Kandah are designing a hybrid testbed for research and testing on autonomous vehicles.

In-vehicle networks are implemented via the ISO standard Controller Area Network (CAN) bus protocol, which is a message-based communication standard for connecting basic, low-powered micro-controllers called Electronic Control Units (ECUs) that are found in modern vehicles. Up to 100 ECUs communicating via the CAN can be found in one vehicle. Likewise, approximately 100 million lines of code can be required to control devices in the network and to keep the vehicle operating properly. CAN is popular throughout the manufacturing automation sector and other sectors other than automobiles such as in medical devices and industrial equipment.

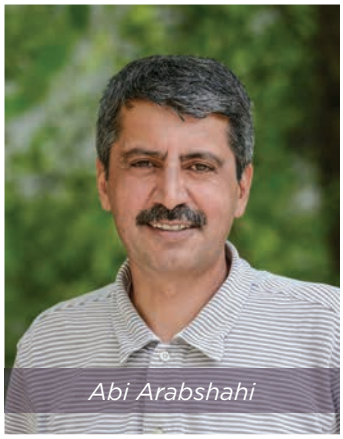
CAN is a broadcast-based, low-cost, lightweight network that is designed for low-power computing devices with small message size and uses a protocol that has small network overhead. The existing CAN network fulfills the requirements for safety and reliability of a vehicle—but not for security. When modern vehicles are inevitably connected to the outside world by Wi-Fi or cellular networks, security issues arise because CAN was designed with no particular security model or architecture in mind. The simplistic design of CAN exposes various security vulnerabilities that can be exploited easily by a hacker in or near the vehicle.

Simulation of Air Flowing through lungs. Image courtesy of Flow Research Lab (flowresearchlab.com)

AI Meets CFD

Numerical simulation of fluids plays an essential role in modeling many physical phenomena, such as aerodynamics, human pulmonary, weather, climate, and plasma physics. Fluids are well described by a set of equations called the Navier–Stokes, but solving these equations at scale remains daunting, limited by the computational cost of resolving the smallest spatiotemporal features. Computational Fluid Dynamics (CFD) is a computationally expensive numerical simulation modeling technology. Furthermore, despite the high accuracy, performing the numerical simulation falls short in providing the required results in a timely manner. To reduce the required computational time, proxy models have been developed in the past several decades. Traditional proxy models are either statistical or mathematical approaches. They were developed to substitute complex numerical simulation while producing a representation of the system at a lower computational cost. However, there are shortcomings associated with these approaches when applied to complex systems.

To expand the utilization and practicality of the SimCenter's in-house CFD models for applications to real-world multi-physics problems, e.g., to predict fluid flow around complex geometries under complicated motion, everything should be done in a timely manner. Our upcoming plans will implement a Smart Proxy technology that is defined as the engineering application of Artificial Intelligence and Machine Learning for CFD simulations. This tool will allow us to tackle problems that are practically impossible to work with using traditional CFD. Smart proxy modeling will replicate the results of complex CFD models with high accuracy without reducing the physics of the models or its resolution in space and time. Unlike the response surface approach, Smart Proxy modeling will replicate the physics of the CFD model simultaneously for all the cells and all the required output variables.

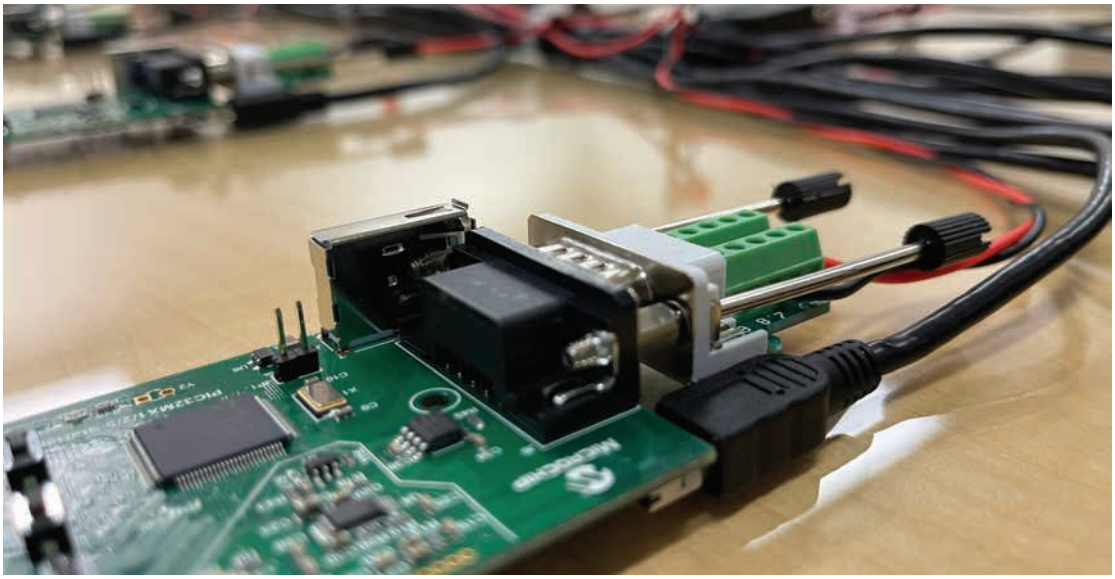


Abi Arabshahi

The smart proxy modeling will be verified and validated through well-established test cases. The first of the selected validation cases will correspond to the aerosolized drug delivery in the human airways where the effects of flowrate, injected particle size, injection distribution on the flow structure and the aerosol deposition fraction on various segments of the airway geometry will be characterized. The setup will use a triple bifurcation lung airway model, which represents 3–6 generations of the human respiratory system. The 3-generation network is a key to biological understanding as the empirical observations have shown a repeated pattern of flows in such fractal branching networks; this is a common biological network exemplified by the human bronchial tree.

XiveNet cont...

XiveNet, the testbed being developed, will comprise both real and simulated ECUs, to eliminate significant costs such as the need to purchase a separate vehicle for testing. The hybrid approach will allow the testbed not only to be flexible but also to mirror real-life scenarios by providing more realistic feedback than a software-based approach can. This project is funded by the National Security Agency.



CRITICAL INFRASTRUCTURE PROTECTION PROGRAM

Vulnerabilities of national and international infrastructure continue to be exposed by natural disasters, human error, and deliberate attacks. Many of these events have directly impacted the Tennessee Valley and Chattanooga: the 2020 Nashville bombing, the 2020 tornadoes, Chattanooga's 2019 major water supply interruption, and the 2008 Coal-Ash Spill. Protecting critical infrastructure (CI) threatened by these events requires strong partnerships among researchers, communities, businesses, and governments. The Department of Homeland Security (DHS) currently recognizes 16 CI sectors: chemical, commercial facilities, communications, critical manufacturing, dams, defense industrial base, emergency services, energy, food & agriculture, healthcare & public health, information technology, transportation systems, water & wastewater systems.

THE CIP THRUST is led by Dr. Don Reising, Associate Professor in Electrical Engineering. His interest in critical infrastructure began in his master's program and continued through his 18-year military career. He is currently focused on anomaly detection and machine learning in smart power grids.

ON CIP POSSIBILITIES: "Power utilities and water utilities collect a ton of data they may not have time to analyze. I want to find out what happens if one of those data points is associated with somebody doing something malicious on the distribution network, and what we can do about it."

ON THE GOALS OF CIP: "I see it as national security, national defense. It's not putting kinetic weapons on targets, but it's protecting an infrastructure that if an adversary decides to leverage a vulnerability in it, they could really hurt us."

ON SIMCENTER SUPPORT: "Dr. Skjellum's strength is in connecting faculty across silos, leveraging their specific expertise to solve problems they might not otherwise know how to. We couldn't have this thrust otherwise."

A SimCenter-led survey of 26 faculty found eight areas of ongoing or nascent work in CIP at UTC, as well as strong possibilities for growth in six more. This level of engagement, paired with existing partnerships, demonstrates a strong foundation for competitiveness, success, and significant outcomes in CIP at UTC. However, a crucial finding of the survey was that faculty are not typically aware of other CIP work across the university. Interested faculty represent a range of disciplines, including Management, Computer Science, Electrical Engineering, and Nursing; cohering these efforts for meaningful impact will require central coordination.

As a response to recent infrastructure threats and the need for more centralized collaboration, the UTC SimCenter has created a research thrust to support multidisciplinary CIP activities. Led by Dr. Don Reising (Associate Professor of Electrical Engineering) and supported by Dr. Anthony Skjellum (SimCenter Director & Professor of Computer Science), this thrust aims to catalyze new collaborations in CIP, encourage innovation, and connect projects and personnel with resources they require. Recent partners and sponsors of CIP work at UTC include local, regional, state, and national companies and government agencies/ organizations .

The research thrust aims to expand to a standalone center-style organization. The strategic goal of the CIP Center will be to create and leverage local and regional partnerships to expand into six additional CI sectors, for a total of 14. Initial goals include supporting applied research, advanced development, grant proposals, and technology transfer. With such support, a CIP Center at UTC can seek national center-type standing with federal agencies such as DHS, DOD, and NSF. Substantial economic benefits will accrue from the enhanced stature of this future CIP center's outcomes, together with the practical results shared in open source format, through technology transfer, and via traditional scholarly venues.

LAKMALI WEERASENA is an Assistant Professor of Mathematics at UTC. She received her PhD and MS in Mathematical Sciences from Clemson University, and her BS in Mathematics from the University of Peradeniya, Sri Lanka. Her primary research area centers on a more profound understanding of approximation methods in multiobjective combinatorial optimization (MOCO). Her second area of research interest is in bridging optimization theory and applications, particularly in mathematical and engineering sciences, operations management, and conservation biology.

This feature offers a look into Dr. Weerasena's SimCenter-related research in FY2021, as well as a preview of her continuing work from FY2022 onward.

What was your main research focus in FY2021, whether related to the SimCenter or not?

I develop approximation algorithms for multi-objective combinatorial problems and develop mathematical models for conservation biology/invasive species management and emergency services management. This work is a continuation of my study of the multiobjective set-covering problem, a severely understudied problem in my field.

How did the SimCenter factor into your work in FY2021?

I frequently used SimCenter computing facilities for my research work. SimCenter cluster computer facilities were helpful for me to analyze real large-scale data of the invasive species of conservation land in Chattanooga at Reflection Riding Arboretum and Nature Center. I also received support from the SimCenter to resubmit my NSF CAREER proposal and an NSF LEAPS proposal.

What key research collaborations did you begin or continue in FY2021 as a result of SimCenter connections?

I have worked with Dr. Tony Skjellum and Dr. Ryan Marshall (Computational Science postdoc) to develop a parallel meta-solver for the multi-objective set covering problem. In our published paper, we present a serial version of the meta-solver with a novel search procedure that outperforms a previous implementation, and when parallelization techniques are applied, a 9-12x speedup is achieved with the possibility of further improvement for large problems.

I also worked with Dr. Tony Skjellum and Dr. Aniekan Ebiefung (Department of Mathematics) to design an approximation algorithm for the generalized multi-objective set covering problem. In our pending publication, we propose a mathematically driven heuristic algorithm, which uses a branching approach of the feasible region to approximate the Pareto set of the GMOSCP.

How did you include students in your (SimCenter-related) research in FY2021?

Diem Vu, an MCDA student (Master of Science in Data Analytics Program) in the College of Business contributed to exploring the science of multi-objective covering models. In particular, she supported developing a mathematically driven decision-making tool for optimally controlling the invasive species of conservation land in Chattanooga at Reflection Riding Arboretum and Nature Center as a part of a collaborative project. She used SimCenter cluster computing very often for computational work.

What are your plans for continued SimCenter-related research in FY2021 and beyond?

I plan to develop a new research direction connecting machine learning and multi-objective optimization. For this project, I will continue my collaboration with Dr. Tony Skjellum, drawing on his expertise in machine learning.

YU LIANG is a Professor of Computer Science and Engineering at UTC. He received his BE in computer science and technology from Tsinghua University, Beijing, China; his MS in computer science from Beijing University of Technology, Beijing; his first PhD in computer science from the Institute of Computing Technology of Chinese Academy of Sciences, Beijing, China; and his second PhD in applied mathematics from the University of Ulster at Coleraine, Northern Ireland, U.K. Dr. Liang's current research interests focus on modeling and simulation, machine learning and artificial intelligence, big-data and cloud computing, high performance computing, numerical linear algebra, and computational science.

This feature offers a look into Dr. Liang"s SimCenter-related research in FY2021, as well as a preview of his continuing work from FY2022 onward.

What was your main research focus in FY2021, whether connected to the SimCenter or not?

Using Graph-based Motion Analysis to Promote Physical Activity – As a graph-based motion analysis system, the addressed framework converts the motion analysis into graph analysis. This conversion allows powerful graph-based computational tools, e.g., GNNs, to analyze human movements. These tools can automatically extract kinetic patterns by taking advantage of the large amount of preliminary data analysis.

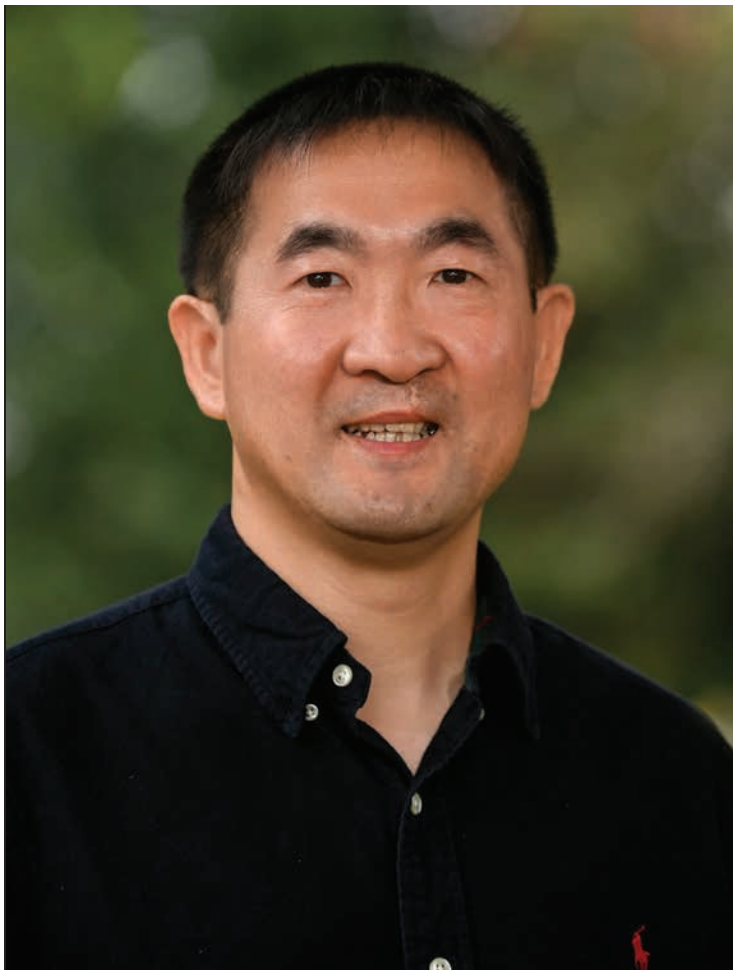
Real-time Subsurface Sensing with Cognitive Robotic Networked System – the overall goal of the project is to create dramatically faster and more accurate subsurface sensing systems with teams of coordinated autonomous cognitive ground penetrating radars (GPRs).

Sensitivity Analysis of Graph Neural Network – This project focuses on investigating the relation between the sensitivity and the architecture of graph neural network.

Applying the Graph Neural Network Approach to Assess the Effectiveness of COVID-19 Vaccinations Across Socioeconomic and Physiologic Strata – This project applies Graph neural networks in the quantitative assessment of the effectiveness of available vaccines (e.g., Pfizer and Moderna) against COVID-19 pandemics. The GNN model will be validated using the Susceptible-Infective-Recovered (SIR) epidemic model with vaccination as ground truth.

How did the SimCenter factor into your work in FY2021?

All above projects are data and computation intensive. We need the technique support of a high-performance computing platform. From the SimCenter, we also received a lot of information about funding opportunities, conferences, training opportunities, and the recent progress of cutting-edge technologies.



What key research collaborations did you begin or continue in FY2021 as a result of SimCenter connections?

Drs. Anthony Skjellum and Ward set up a GPU cluster account for my students so that they can complete their projects.

How did you include students in your (SimCenter-related) research in FY2021?

I divided my students into multiple groups, each of which is led by a senior or PhD student. Therefore the fresh research assistant can get used to the research work very quickly.

What are your plans for continued SimCenter-related research in FY2021 and beyond?

I will strengthen the collaboration with the colleagues in SimCenter, particularly through information exchange about the application of high-performance computing on data processing and analysis.

LOREN HAYES is an Associate Professor in Biology, Geology, and Environmental Science. He received hi BS in Biology from Bates College, his MS in Zoology from Michigan State University, and his PhD in Zoology from Miami University. The aim of his research program is to better understand why some species live in groups and rear offspring communally. His work has an international theme, with collaborators in various countries including Chile, Colombia, France, Switzerland, and the U.S.

This feature offers a look into Dr. Hayes' SimCenter-related research in FY2021, as well as a preview of his continuing work from FY2022 onward.

What was your main research focus in FY2021, whether connected to the SimCenter or not?

Mammalian social evolution: In collaboration with Dr. Carsten Schradin's research group at CNRS-Strasbourg (France), my lab group collected data on the social organization of whales and life history data on artiodactyls. We added these data to a large dataset on all mammals. Related to this work, my research group is collaborating with Drs. Jin Wang (UTC - Math) and Azad Hossain (UTC – BGE) to model the effects of rainfall and lifespan on the prevalence of variable social organization within populations.

How did the SimCenter factor into your work in FY2021?

Funding supported a graduate student project on artiodactyl lifespans. My student collected data on lifespan from the primary literature and compared these results to data in online datasets. This is an important first step to determining which dataset to use in phylogenetic (evolutionary) comparisons.

What key research collaborations did you begin or continue in FY2021 as a result of SimCenter connections?

Dr. Azad Hossain (BGE) will collect rainfall data from an online dataset for our mammalian database. This information will be used in an analysis to determine how rainfall influences the evolution of social organization in mammals. Dr. Jin Wang (Math) and a student will run mathematical models to determine how environmental conditions influence variation in social organization within populations.

How did you include students in your (SimCenter-related) research in FY2021?

(1) Environmental Science Masters student. Project: Life history drivers of artiodactyl social organization (2020-21)

(2) Geology undergraduate student (Hossain). Project: Collecting rainfall data (Summer 2021)

(3) Math student (Wang). Project: Modeling effects of rainfall and lifespan on social organization (summer 2021)

(4) BGE undergraduate student. Project: Collecting data on group size

What are your plans for continued SimCenter-related research in FY2021 and beyond?

I plan to maintain a collaboration with Dr. Carsten Schradin (CNRS France) that started in 2015. Our research aim is to understand how rainfall and life history influence the evolution of social organization. This collaboration will involve student-student and faculty-student collaborations. For example, Dr. Schradin participated as a mentor in my NSF IRES program in summer 2021. He supervised a project by a UTC undergraduate student. Long term (10 years), we hope to examine factors contributing to variation in mammalian social organization, mating systems, and parental care.

JENNIFER BOYD is an Associate Professor of Biology, Geology, and Environmental Science at UTC. She earned a Ph.D. in Earth and Environmental Sciences with a concentration in Ecology from Columbia University in 2003. Her undergraduate degree is in Environmental Science and English (double major) from Allegheny College (Meadville, PA). She is a plant ecologist, and her research focuses on rare species. She is especially interested in the factors that influence species rarity and commonness and the vulnerability of rare versus common species to environmental change.

This feature offers a look into Dr. Boyd's SimCenter-related research in FY2021, as well as a preview of her continuing work from FY2022 onward.

What was your main research focus in FY2021, whether connected to the SimCenter or not?

My main research focus in FY2021 was to continue my ongoing work investigating the potential for rare species to be constrained by limited abilities to adapt and acclimate to environmental change. This work is supported by a Population and Community Ecology Core award from the NSF Division of Environmental Biology and involves collaborators from the University of Georgia, University of Oxford, Austin Peay State University, and Seton Hall University. My major activities during FY2021 involved (1) synthesizing the literature on plant species rarity with focus on the integration of ecological and evolutionary concept with network analysis, and (2) conducting empirical experiments with two parts of rare and common congeneric species in growth chambers to compare their abilities to acclimate to environmental change. Our network analysis project was published in Ecology and Evolution in August 2020 and the empirical work is currently in review for publication.

How did the SimCenter factor into your work in FY2021?

The network analysis project described above involved collaboration (and co-authorship) by SimCenter faculty (Dr. Craig Tanis). We used computational tools to search and characterize a large literature base in ways that were outside of my area of expertise as an ecologist.

What key research collaborations did you begin or continue in FY2021 as a result of SimCenter connections?

I am currently collaborating on a somewhat analogous but more expanded network analysis project with Dr. Hope Klug (BGE) and the SimCenter to characterize research on sexual selection. I am also discussing the potential to develop a collaborative research proposal with Dr. Klug that includes computational work – possibly an NSF REU.

How did you include students in your (SimCenter-related) research in FY2021?

A UTC UHON student, Thomas Wiegand, was the lead author of the network analysis project described above. Another student in BGE, Braley Gentry, was a co-author. Thomas continues to work in my lab now as an MS in Environmental Science graduate student. Recently, he was awarded a prestigious NSF Graduate Research Fellowship Program (GRFP) award to study rarity in sunflowers and conduct a related meta-analysis that will utilize SimCenter resources.

What are your plans for continued SimCenter-related research in FY2021 and beyond?

I will soon be focusing on writing a grant proposal to the NSF Population and Community Ecology Core program that will include a computational component. I also will continue collaboration with Dr. Klug on her sexual selection network analysis project in conjunction with the SimCenter.

STUDENT PROFILES

DALLAS JONES I have an Associate's Degree of Science in General Studies. Currently, I am completing a BS in Mechanical Engineering. I am employed under Dr. Anthony Skjellum.

My current internship involves me working with Dr. Skjellum and, namely, learning commands in the coding language Python and how to more quickly carry out certain tasks using Python. My first research project focused on image processing using Python. I learned about what algorithms are used in Python to process images, as well as how startup times for processing images are calculated. I have started to expand this project with Dr. Anthony Skjellum, Sai Medury, and Derek Schafer.

During my college career, at the undergraduate level, I plan to continue my research in Python and other coding languages. After graduation, I would like to enter a career that implements my knowledge of Python and the other coding languages I've learned, such as HTML, CSS, and others. I would also be open to having a career in Engineering Design, using the knowledge I have acquired during my undergraduate, and possible graduate, academic career.

SAI MEDURY I'm working towards my PhD in Computational Science and my educational background is Computer Science Engineering. I also completed an MS in Software Engineering at Auburn University in 2017. My adviser is Dr. Anthony Skjellum, and I also collaborated with Dr. Farah Kandah in the past year.

I have had two internships in the past couple of years. The first was at Autodesk in San Rafael, CA, in 2019, where I worked as a Blockchain Researcher Intern. In this internship, I explored Distributed Ledger Technology-based Identity Management for Export Compliance use cases for validating customer identity and screening against global watchlists. I also developed a whitepaper describing research and analysis, recommending a roadmap for implementing Distributed Ledger Technology-based customer identity management in production.

My second internship, in 2019 and 2020, was with Branch Technology in Chattanooga as a Software Engineering Intern. The position was funded by an NSF Supplemental Funding grant. I developed a feature to automate the process of identifying 3D blocks with custom specs among a set of spatial coordinates in CAD models. I optimized execution of this new feature by performance profiling, and revised bottle-neck areas of code. I also set up a CMake-based build system in alignment with the team's DevOps workflow.

Finally, I configured Bamboo-based Automated testing and Continuous Delivery for projects written in C++ and C#.

In FY2021, I focused on leveraging blockchain technology to build more secure and robust systems. In collaboration with Amani Altarawneh and my advisor, Anthony Skjellum, I designed and published the Cascading Cuckoo filter, a set-membership data structure that produces zero-false-positives. It was also awarded the best paper in the category of File and Storage Systems at the 11th Annual Computing and Communication Workshop and Conference (CCWC).

Dr. Skjellum and I also worked with Ilker Ozcelik and Tanner Broaddus on preparing an Overview of Crypto Accumulators that includes a primer to understanding crypto-accumulators and their properties. Further, we reviewed literature, proposed a taxonomy for classifying constructions so far, and presented technical insights to guide developers through the process of choosing the right construction for an application.

Dr. Skjellum and I also collaborated with Dr. Nishani Vincent from UTC Business school to design and publish a blockchain-based architecture to help CPA firms. This architecture helps facilitate effective connectivity to a blockchain while enabling auditors to leverage this technology to provide audit and assurance services.

Conner Fulford, Amani Altarawneh, Anthony Skjellum, and I are working on designing a time synchronization to be applied in peer-to-peer distributed computing environments. This algorithm enables peers in a decentralized computing environment to synchronize time with each other. This research work is currently in progress and is expected to be published by September 2021. I'm planning to graduate in Fall 2021 and seeking system engineering opportunities in research computing environments.

STUDENT PROFILES

EVELYN NAMUGWANYA I have a BS in Information Technology from Makerere University - Uganda and a certificate in CISCO Networks. I recently completed an MS in Computer Science at UTC. I work with Dr. Skjellum as a research assistant, and he is my advisor.

My research is about data redistribution, developing a high-level API that works directly with the Message Passing Interface (MPI) to redistribute Linear Algebra libraries such as polymath.

The goal is to observe performance trends and analyze results based on the cost of redistribution and determine whether it pays off to redistribute data for large problem sizes.

The SimCenter has enabled me to have a meaningful and excellent education and research experience at UTC. The SimCenter has provided conducive working space and apparatus for our research. We run most of our experimental tests using Cluster 117, and this is a powerful machine.

I will soon begin my PhD in Computational Science in Fall 2021 at UTC. I will still work with Dr. Skjellum on research in High-Performance Computing and further improve my Master's research about data redistribution and optimization of parallel linear algebra libraries.

BRENNAN HUBER I obtained my BS in Computer Science: Scientific Applications & my MS in Computer Science: Cyber Security, both from UTC. I am currently pursuing a PhD in Computer Science, under my advisor Dr. Farah Kandah.

I had my first internship my 3rd year of my undergraduate degree. It was at BlueCross BlueShield of Tennessee serving as a project management intern. I had no idea what I wanted to do as a career, and I wanted to get experience while also being able to see a bunch of different areas to find what I wanted to work on. Since then, that internship has converted to a full-time position where I have moved positions a couple of different times, from working on database queries to build ad hoc reports for leadership. Now I mostly spend my time rewriting old COBOL programs into C# to eliminate some technical debt that our team has.

In my research, I have teamed up with Tennessee Tech University to work on a NSF funded project called XiveNet, where we are focusing on the security of the control units of vehicles. Another project that we are pursuing is the extension of my MS thesis work, which has to do with furthering Trust Management to include deep learning such that it is possible to monitor the data that devices are sending instead of relying on a consensus as in traditional trust management schemes. The last project I am on is writing a survey paper. The team I am a part of works with security, primarily of IoT devices, and we are currently working to review tons of papers such that we are able to build a universal threat model. By identifying current areas that lack research, we will be more able to fill those gaps in the future.

The SimCenter has been directly related to all of my previous projects. The thing about the SimCenter that wasn't captured in my project descriptions is the people who are there. Everyone is so incredibly helpful and interested that you can spark up a conversation with anyone and obtain feedback immediately. This type of collaboration is one of the best aspects of the SimCenter.

Though Dr. Kandah is my primary advisor, we have been collaborating with Dr. Skjellum and his team since day one. Our teams have a lot of overlap, so we are able to have stimulating discussions on how the project will work and what potential downfalls there are.

I am currently finishing up my coursework and beginning my focused research and dissertation. I will be continuing my job at BlueCross BlueShield, but upon graduation I am really hoping to find a faculty position at a university. I really enjoy research and I look forward to being able to pursue any path that piques my interest later in life. Further, I always wanted to be a teacher and since I have found my passion in computer science I hope to be able to share the information and maybe spark a passion for someone else.

STUDENT PROFILES

MAXWELL OMWENGA I graduated from Makerere University - Uganda in 2006 with a BS in Computer Science and in 2012 with an MS in Data Communication and Software Engineering. I have recently completed my PhD in Computer Science at UTC. My doctoral dissertation was conducted under the tutelage of Dr. Dalei Wu and Dr. Liang Yu.

After my undergraduate studies I worked as a web administrator at Makerere University for 7 years and worked at Bugema University as a lecturer for 2 years. For the past 5 years I have worked as a graduate research assistant at UTC in the networked intelligence lab funded by NSF.

My main research focus was three-fold. The first goal was to establish reinforcement learning architectures for intelligent cognitive GPR sensing. The second was to develop a delay sensitive fog computing framework, capable of supporting service migration for mobile Internet of Things (IoT) devices. Finally, I worked to extend the local approach for the detection and recognition of subsurface objects to a global approach through a novel 3D scan cloud.

The SimCenter super computing infrastructure has been a great resource for me to train and test my machine learning models. With limited ground truth data of subsurface objects, a generative adversarial network model architecture to synthesize realistic datasets was implemented, since model performance in machine learning is heavily dependent upon the availability of training data. Also, by formulating the cognitive subsurface object detection as a Markov decision problem (MDP), a deep reinforcement learning framework was established to resolve the problem by implementing algorithms with novel reward functions that combines intermediate rewards from both region-of-interest (RoI) identification, object classification, and object reconstruction. Simulation results, i.e. performance accuracy and robustness, were carried out on the TS supercomputer. I continued with the subsurface infrastructure mapping for smart cities project in the networked intelligence lab under Dr. Dalei Wu and Dr. Yu Liang.

I am looking forward to a data science position with a forward-looking technology company, where I intend to work for a few years and become a seasoned data scientist, then later join academia as a way to give back to the community by encouraging and promoting STEM programs.

THOMAS WIEGAND I graduated from UTC with my BS in Environmental Science and BA in French Language and Culture in December 2020. In January 2021, I started the MS in Environmental Science program at UTC. I work for Dr. Jennifer Boyd and have previously worked with Dr. Hope Klug and Dr. Craig Tanis.

My main research focus in FY2021 was investigating the potential importance of plasticity to plant species rarity through controlled growth chamber experiments with closely-related rare and common plant species. Our two most recent experiments investigated the plastic responses of growth and allocation traits in rare and common species of Xyris and Scutellaria when subjected to different environmental treatments.

During FY2021, I completed a collaborative project with Drs. Jennifer Boyd, Hope Klug, and Craig Tanis where we used network analysis to illustrate connections between ecological and evolutionary concepts in studies of plant rarity over the past ~30 years. Dr. Tanis's expertise with text-mining aided tremendously in this project, which culminated in a publication in Ecology and Evolution in August. This is the largest-scale conceptual review of plant rarity studies published to date and an example of a unique use of network analysis. As a continuation of this project, I have worked with Dr. Hope Klug and Dr. Jennifer Boyd to conceptualize a project where we will use these same methods to illustrate the conceptual framework of studies related to sexual selection.

I was recently named a recipient of the National Science Foundation's Graduate Research Fellowship. I will complete my master's in environmental science at UTC before pursuing my PhD in a related field. In addition to my research at UTC, I will conduct a large-scale growth experiment with sunflower species of various geographic distributions in cooperation with a team at the University of Georgia and the State Botanical Garden of Georgia.

I will also be working in community outreach for young queer students interested in science in Chattanooga and local Native American students during my time at the University of Georgia. I plan to pursue a PhD in plant ecology or a related field, as I am interested in a career centered around the conservation of rare species.

RECENT UPDATES


Dr. Amani Altarawneh

DR. AMANI ALTARAWNEH was the first female graduate of the Computational Science PhD at UTC, in May 2021. She has accepted an Assistant Professor position at Colorado State University.

RYAN MARSHALL, former postdoctoral associate under. Dr. Tony Skjellum, has taken a position at the University of Alabama.

FOUR STUDENTS completed internships at Department of Energy national laboratories in FY2021: Grace Nansamba (LLNL), Tanner Broaddus (LANL), Carson Woods (SNL), and Tom Herschberg (LANL).

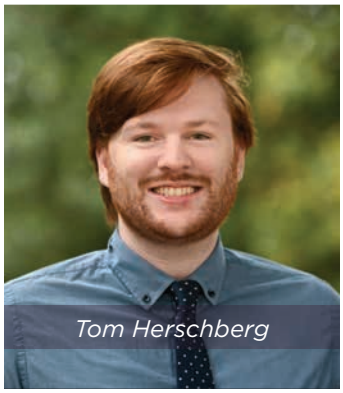
DR. TONY SKJELLUM worked with five undergraduate students over the summer, funded by the National Science Foundation Research Experiences for Undergraduates program: Clara Alsobrooks, William Garrett Hooten, Alex Hershberg, Dallas Jones, and Connor Fulford.

Dr. Bruce Hilbert

BRANCH TECHNOLOGY, where alum Dr. Bruce Hilbert serves as Director of Software Engineering, has constructed the first-ever 3D-printed building facade for the Tennessee Valley Federal Credit Union branch located on W. 20th St. in Chattanooga.

MARTIN RUEFENACHT, former research associate under Dr. Tony Skjellum, has taken a position at the Leibniz Supercomputing Centre of the Bavarian Academy of Sciences and Humanities (LRZ) in Munich.


Martin Ruefenacht


Tom Herschberg

TOM HERSCHBERG graduated with his BS in Computer Science and is going on to pursue his PhD at the University of Illinois at Urbana-Champaign.

IN MEMORIAM

DR. HENRY "HARRY" MCDONALD passed away in May 2021. While at UTC, Dr. McDonald held the Chair of Excellence in Computational Engineering. He established the THEC Center of Excellence in Applied Computational Science and Engineering and helped secure approval for UTC's first PhD program in Computational Engineering.

FUNDED PROPOSALS IN FY2021

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. 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. 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 10 following SimCenter-affiliated proposals were funded in FY2020, for a total of $1,053,469.

Title	PI	Funding Agency	Amount
REU Supplement for SPX: Collaborative Research: Intelligent Communication Fabrics to Facilitate Extreme Scale Computing	Dr. Tony Skjellum	National Science Foundation (NSF)	$16,000
REU Supplement for CC* Compute: A Cost-Effective, 2,048 Core InfiniBand Cluster at UTC for Campus Research and Education	Dr. Tony Skjellum	NSF	$16,000
Hypersonic Vehicle Structure Critical Technology Gaps	Dr. James Newman	University of Dayton Research Institute	$535,125
REU Supplement for CC* Networking Infrastructure: Advancing High-speed Networking at UTC for Research and Educations	Dr. Farah Kandah	NSF	$16,000
Supplement for SHF: Medium: Collaborative Research: Next-Generation Message Passing for Parallel Programming: Resiliency, Time-to-Solution, Performance-Portability, Scalability, and QoS	Dr. Tony Skjellum	NSF	$103,537
C++ API for Checkpoint/Restart for MPI Applicatiosn	Dr. Tony Skjellum	Lawrence Livermore National Laboratory	$60,824
Safer Power Network	Dr. Don Reising	State of Tennessee RevV!	$100,000
XiveNet: An Extensible, Innovative, and Open Architecture Testbed for In-Vehicle Network Security Research	Dr. Farah Kandah	National Security Agency	$51,003
Exploiting Metallohinged Trans-bidentate ligands for Suzuki Coupling	Dr. Jared Pienkos	American Chemical Society Petroleum Research Fund	$55,000
Learning from Power Signals	Dr. Don Reising	Tennessee Valley Authority	$99,980

SELECTED FY2021 PUBLICATIONS AND PRESENTATIONS

CONFERENCE PRESENTATIONS, POSTERS, AND PROCEEDINGS

Assessment of Subgrid Dispersion Models for Large-Eddy Simulation of Particle-Laden Turbulent Flows, AIAA Scitech, 2021. (**Abdollah (Abi) Arabshahi**)

"Predicting Steam-Gasification Output Using Artificial Neural Networks" has been accepted for IMECE 2021 for both publication and conference presentations. (**Yunye Shi**)

Q. Baldwin, Applied Knot Theory Workshop 2020, UTC (**Eleni Panagiotou**)

Q. Baldwin, AMS Southeastern Fall Sectional meeting 2020, Contributed Session, UTC (**Eleni Panagiotou**)

E. Panagiotou, BMSE/MCDB joint seminar, UCSB

Q. Baldwin, Research Dialogues 2021, UTC, (**Eleni Panagiotou**)

Arielle Beard and Achok Alier, Research Dialogues 2021, UTC (**Eleni Panagiotou**)

Bailey, A. & Smith, A. (2021). Of parks and pandemics: Visitation disparities across county lines. Presentation for the Southeastern Recreation Research Conference (virtual, refereed); March, 2021

Bailey, A. & Smith, A. (2021). Of parks and pandemics: Visitation disparities across county lines. Presentation for UTC Research Dialogues (virtual); March, 2021

Bailey, A., Heath, G.W., & Mix, Charlie (2021). People, Planet, & Profits: Strategic planning for outdoor recreation, tourism, and conservation (virtual). A CEACSE presentation for UTC Research Dialogues; March, 2021

Application of Intrusive and Non-Intrusive Reduced Order Modeling Techniques for Simulation of Turbulent Premixed Flames, AIAA Propulsion and Energy Forum and Exposition, 2021 (Presenter: **R. Ranjan**).

Application of Hybrid Transported-Tabulated Chemistry for Efficient Large Eddy Simulation of Turbulent Premixed Combustion, AIAA SciTech Forum and Exposition, 2021 (Presenter: **R. Ranjan**).

Numerical Investigation of the Effects of Elevated Pressure and Chemistry on the Characteristics of Turbulent Premixed Flames, Research Dialogues, UTC, 2021 (Presenter: J Bowers). (**Reetesh Ranjan**)

Simulation of Extinction And Re-Ignition Events in a Turbulent Non-Premixed Flame, CECS Tech Symposium, UTC, 2021 (Presenter: J. Doshi). (**Reetesh Ranjan**)

Effect of Pressure on Heat Release and Curvature Statistics of Turbulent Premixed Flame, CECS Tech Symposium, UTC, 2021 (Presenter: J Bowers). (**Reetesh Ranjan**)

Large Eddy Simulation of the Volvo Bluff Body Flame Experiment, CECS Tech Symposium, UTC, 2021 (Presenter: E. Durant). (**Reetesh Ranjan**)

Suggs, E.D. 2019. Meta-textual analysis of biological research. ACM meeting, Gatlinburg, TN. (**Loren Hayes**)

Miles, M. Variable social organization is ubiquitous in Artiodactyla and probably evolved from pair-living ancestors. Summer 2020, presentation to **Hayes**, Schradin (France), and Fernandez-Duque (Yale) lab groups.

Hayes, L. D., Miles, M., Pope, E., and Schradin, S. Artiodactyl social organization: Explaining the evolution of variability. 2021 UTC Research Dialogues.

P. Ubiratan, S. Wasti, and **V. Disfani**, "Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm," in 2020 IEEE International Conference on Smart Grid Communications (SmartGridComm), IEEE, 2020.

P. Ubiratan, S.Wasti, and **V. Disfani**, "Frequency Deviation Controller for Inter-Area Oscillations Damping in Smart Grids," in 2021 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT), IEEE, 2021.

P. Ubiratan, "Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021. (**Vahid Disfani**)

Oral presentation scheduled at the Solar Energy Systems Conference, AlChE, 2021. (**Sungwoo Yang**)

Oral talk at Materials Research Society Annual Conference, Virtual Meet, 2020. (**Sou Palchoudhury**)

Biophysical analysis of SARS-CoV-2 transmission and theranostic development via N protein computational characterization. Biotechnology Progress (Accepted for publication) (**Michael Danquah**)

Engineered Aptamers for Enhanced COVID-19 Theranostics. Cellular and Molecular Bioengineering (Under Review) (**Michael Danquah**)

SOFTWARE

VF-LESLIE: A fully compressible multi-species reacting flow solver **(Reetesh Ranjan**)

UTCFOAM: In-house and extended version of OpenFOAM (**Reetesh Ranjan**)

REFEREED PUBLICATIONS

A paper entitled "Predicting Steam-Gasification Output via Machine Learning Approaches" is under review in Energy. (**Yunye Shi**)

Baldwin, Q. and **Panagiotou E.**, 2021, The local topological free energy of proteins Journal of Theoretical Biology (under minor revision)

Baldwin, Q., Sumpter, B. G. and **Panagiotou E.**, 2021, The local topological free energy of the SARS-CoV-2 spike protein (submitted-under revision)

Panagiotou, E., Vuong, V. Q., Irle, S. and Sumpter, B. G., 2021, Geometry as a screening tool for strong binders to the SARS-CoV-2 Spike protein (submitted)

J. Bowers, E. Durant, and **R. Ranjan**, "Application of Intrusive and Non-Intrusive Reduced Order Modeling Techniques for Simulation of Turbulent Premixed Flames", AIAA-2021-3634.

V. Hasti and **R. Ranjan**, "Analysis of Flame Structure During Longitudinal Combustion Instability within a High-Pressure Shear Coaxial Single Element Combustor", Accepted for Symposium on Thermoacoustics in Combustion: Industry meets Academia (SoTiC 2021), 2021.

J. Bowers, E. Durant, and **R. Ranjan**, "On the Effects of Variation of Pressure, and Length- and Velocity-Scale Ratios on the Features of Methane/Air Turbulent Premixed Flames", Under Preparation, 2021.

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P. Ubiratan, S. Wasti, and **V. Disfani**, "Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm," in 2020 IEEE International Conference on Smart Grid Communications (SmartGridComm), IEEE, 2020.

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P. Ubiratan, "Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021. (**Vahid Disfani**)

High Temperature Stable Aerogel by ALD Coating (in revision) (**Sungwoo Yang**)

Enhanced Solar Receiver Efficiency Using Superhydrophobic Cost-Effective Ambiently Dried Aerogel (in progress, 50%) (**Sungwoo Yang**)

PATENT APPLICATIONS

Cheap, strong, waterproof, optically transparent, thermally insulating retrofit (**Sungwoo Yang**)

Novel Silica Precursor to Synthesize Ambiently Dried Transparent Aerogel (**Sungwoo Yang**)

Novel Air Burning Method to Synthesize Transparent Insulator (**Sungwoo Yang**)

SIMCENTER STAFF

Left to Right: Holley Beeland, Anna Lane, Kim Sapp, Tony Skjellum, Mike Ward, and Bailey Kirby (Chris Dowell not pictured)

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.

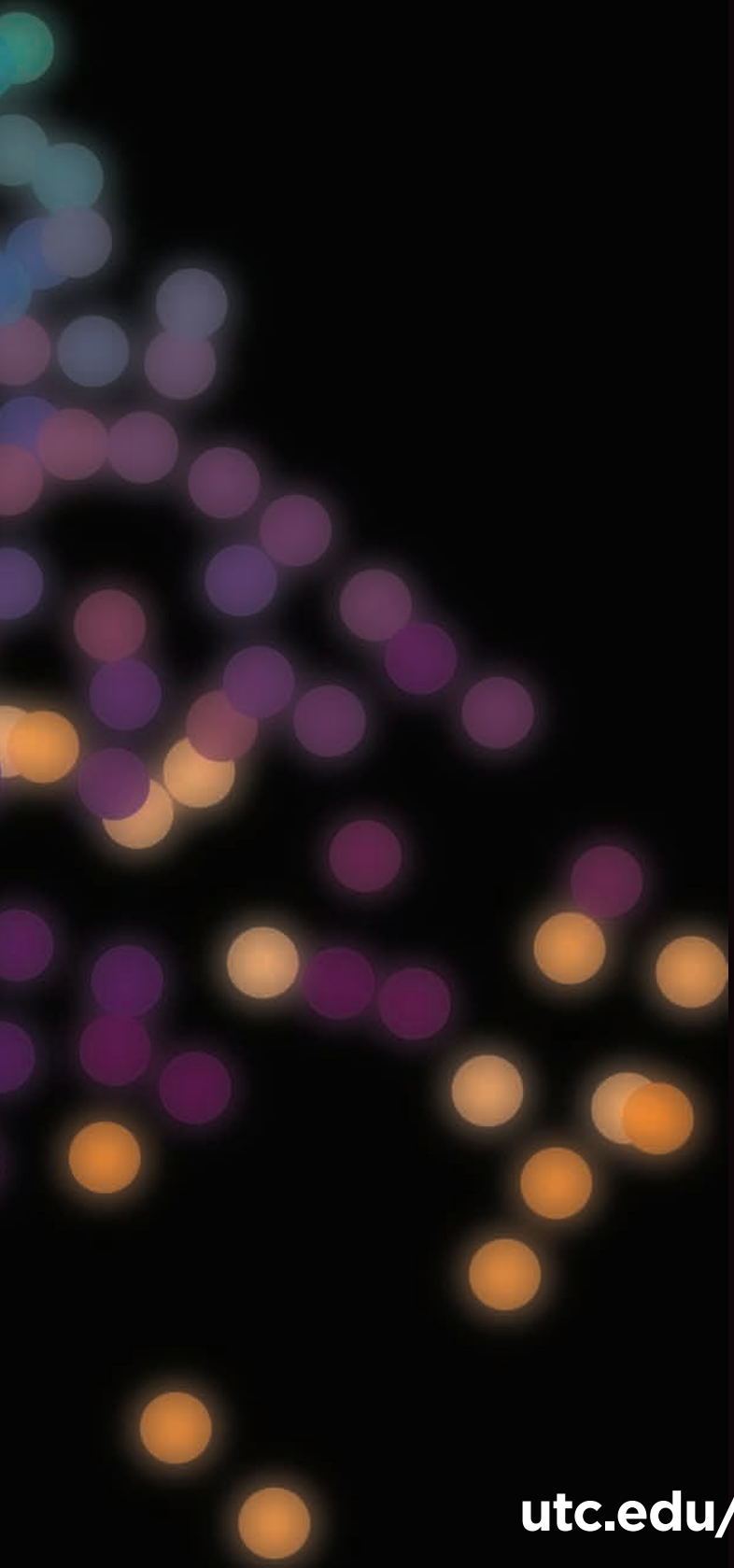
CHRIS DOWELL *(not pictured)* has a 20+ yr IT history working for companies such as Lexmark, IBM and Oracle. He recently moved to Chattanooga from Bozeman, MT. Chris lends his expertise to all SimCenter students and projects as one of the primary High-Performance Computing System Administrators in the Multidisciplinary Research Building. His work is focused on helping users orient to a clustered computing environment and on solving their technical issues while improving and maintaining the existing computing infrastructure.

BAILEY KIRBY joined UTC in March 2018. As the Grant 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.

DR. MICHAEL WARD earned his EdD in Educational Leadership at UTC in 2003. Upon completion, he was hired as a Network Technician. Since that time, he has worked in other roles such as System Administrator and Security Analyst. He has also been adjunct faculty for Computer Science and Education since 2000. As the Cyber Infrastructure Facilitator in the SimCenter, he helps to maintain and organize the HPC infrastructure while facilitating the use of that infrastructure.



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