SimCenter

Center of Excellence in Applied Computational Science and Engineering

2019-2020 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 2020 (July 1, 2019–June 30, 2020). 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 program at UTC, 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.

During FY2020, we reorganized our existing research thrusts to include eight specific areas: Advanced Modeling and Simulation, Cybersecurity and Cyber-physical Systems, Digital Twins, Energy, Environment, Extreme Systems, Health and Biosystems, and High-Performance Computing and Algorithms. Extreme Systems is the newest, formed just before the end of the fiscal year. We will spend FY2021 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 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.*

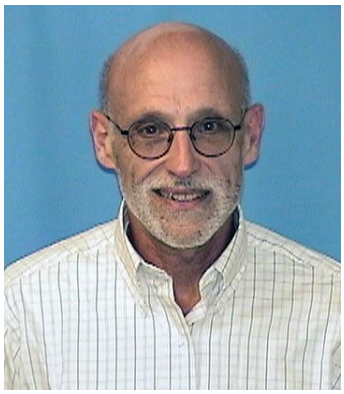
INAUGURAL LEADERSHIP COUNCIL

In June 2020, the SimCenter Leadership Council convened its first annual meeting. The council comprises 11 highly qualified individuals from industry and national lab partners, plus one UTC faculty representative and one UTC student representative. Duties of a Leadership Council member for the two-year inaugural period will include the following:

- Work to finalize the charter for the Leadership Council
- Help to identify opportunities for the SimCenter in your organization and throughout the United States
- Provide input and advice on how the SimCenter can grow and prosper
- Help to advocate at the UT system level, where appropriate, to enhance the SimCenter
- Connect UTC faculty with others to help promote interdisciplinary research across our thrust areas
- Develop an annual report for the benefit of the SimCenter Director, the UTC Vice Chancellor for Research, and the UTC Chancellor that identifies the Council's opinions on how well the SimCenter is doing and where it needs help to further advance the University mission

Ron Brightwell, Sandia

Jeff Cornett, ORNL



Dr. Chris Cox, UTC

Dr. Kate Evans, ORNL

Dr. Bruce Hilbert, Branch Technology

Dr. Barney Maccabe, ORNL

Dr. Kathryn Mohror, LLNL

Dr. Giuseppe Pizzorno, Erlanger & UTCOM

Dr. Howard Pritchard, LANL

Deb Socia, The Enterprise Center

Tom Herschberg, UTC (student)

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 FY2020, the following students from underrepresented groups were 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.

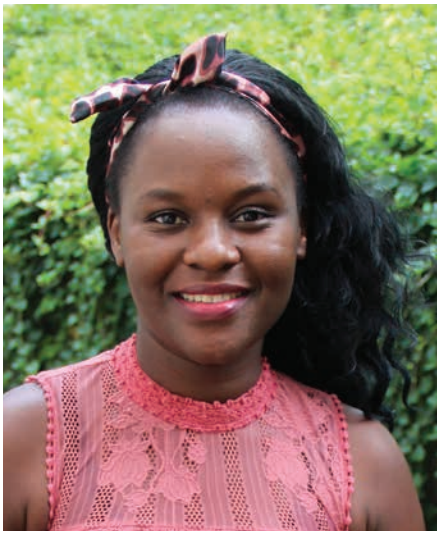
Further recruitment and support sources will include the several ongoing NSF-funded Research Experiences for Undergraduates (REU) projects at UTC, the SimCenter-hosted Middle Tennessee Cyberinfrastructure Alignment Consortium (MTCAC) funded by the NSF Campus Cyberinfrastructure (CC*) program, and the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

Alissa Coleman, MS Electrical Engineering

Crystal Trollinger, BS Computer Science & Engineering

Dallas Jones, BS Mechanical Engineering

Clara Alsobrooks, BS Computer Science & Engineering



Evelyn Namugwanya, MS Computer Science & Engineering

Grace Nansamba, MS Computer Science & Engineering (PhD beginning Spring 2021)

Savannah Camp, MS Computer Science & Engineering

Madison Morris, MS Computer Science & Engineering

Japorsche Pettaway, MA Creative Writing

Sevaughn Orr, BS 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. With our previous report for FY2020, CEACSE marked its 14th 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. This report for FY2020 follows up our previous report with CEACSE's focused priority areas, highlights the ongoing strengths of its visionary leadership team, and notes greater impacts across a range of stakeholder groups. 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), five Initiation/Opportunity Awards ($15,000), and two Lecture Series Grants ($2,500) in FY2020.
- We launched three new research thrusts: Digital Twins (led by Dr. Abi Arabshahi), Extreme Systems (led by Dr. Daniel Loveless), and Advanced Modeling & Simulation (led by Dr. Eleni Panagiotou).
- Dr. Don Reising, leader of the Environment research thrust, received $100,000 from the ORNL/UT/Launch Tennessee RevV! program for a project entitles "Safer Power Network" with Hayden Data Systems
- Drs. Anthony Skjellum and Craig Tanis, leaders of the High-Performance Computing & Algorithms research thrust, received $100,000 from the Sandia National Laboratories for continued studies of Exascale Computing.
- Dr. Anthony Skjellum received $60,000 from the Lawrence Livermore National Laboratory for Fault-Tolerant HPC Research.
- Dr. Anthony Skjellum received $32,000 in REU Supplement funding for existing awards.
- Dr. Farah Kandah, leader of the Cybersecurity & Cyber-physical Systems thrust, received $16,000 in REU Supplement funding for existing awards.
- Dr. Anthony Skjellum received a supplement of $103,537 to his award "SHF: Medium: Collaborative Research: Next-Generation Message Passing for Parallel Programming: Resiliency, Time-to-Solution, Performance-Portability, Scalability, and QoS."
- Drs. Reetesh Ranjan and Abi Arabshahi submitted a proposal to the Department of Defense Investigator-Initiated Research Award competition, for a project related to computational modeling of human airways, especially to be used in treating respiratory infections that result from COVID-19.
- Drs. Reetesh Ranjan, Abi Arabshahi, Trevor Elliott, Henry Spratt, David Levine, Chuck Margraves, and Abudl Ofoli submitted a proposal to the Department of Defense Investigator-Initiated Research Award competition, for a project related to COVID-19 air filtration and sanitizing.
- With CEACSE funds, the SimCenter supported four projects related to COVID-19 research: Dr. Michael Danquah, Dr. Abi Arabshahi, Dr. Soubantika Palchoudhury, and Dr. Eleni Panagiotou. Their work is outlined in the next pages.
- Dr. Anthony Skjellum co-organized, with the University of Tennessee, an exhibitor booth at SC19, a collaboration that is likely to be annual.
- Dr. Anthony Skjellum co-led an Exascale MPI workshop at SC19 (The International Conference for High Performance Computing, Networking, Storage, and Analysis). Other organizers included Sandia National Lab, the EPCC (Edinburgh Parallel Computing Centre, a supercomputing center based at the University of Edinburgh), and the University of Alabama at Birmingham.
- Technical collaborations within the SimCenter led to the creation of the "Advanced Modeling & Simulation" and "Extreme Systems" thrusts in FY2020. The Aerospace and Defense thrust graduated from the SimCenter through its excellence in performing research and securing funding.

- Drs. Anthony Skjellum, Craig Tanis, and Abi Arabshahi received advance authorization to proceed on PSAAP-III funding from the Department of Energy. The 5-year, $4,000,000 award is led by the University of New Mexico.

Some important technical advances

- Dr. Anthony Skjellum co-organized the First Workshop on Compiler-assisted Correctness Checking and Performance Optimization for HPC (C3PO'20), held virtually in June 2020. The workshop brought together researchers with a shared interest in applying compilation and source-to-source translation methodologies to enhance parallel programming, including explicit programming models such as MPI, OpenMP, and hybrid models.
- Drs. Loren Hayes and Craig Tanis collaborated on a predictive modeling project at the intersection of computer science and biology. They developed an automated search platform to obtain papers from the Google Scholar database to help researchers determine whether the stored papers are suitable for a given project. This work led to an NSF proposal to the Integrative Organismal Systems program.
- Drs. Jennifer Boyd and Craig Tanis used network analysis, a tool useful for analyzing connections between parts of a system, in an unconventional way to examine the integration of ecological and evolutionary research foci in studies of plant species rarity. Dr. Boyd's empirical work focuses on the abilities of rare species to acclimate and adapt to environmental change, which involves both ecological and evolutionary processes, so this network analysis helps provide context for her work. This project involved a collaboration between UTC undergraduates Thomas Wiegand and Braley Gentry and former graduate student Zach McCoy; UTC faculty mentors with expertise in ecology (Dr. Jennifer Boyd), evolution (Dr. Hope Klug), and computational methodologies (Dr. Craig Tanis); and a mathematical biologist from the University of Oxford (Dr. Mike Bonsall).
- Drs. Daniel Loveless (leader of the Extreme Systems thrust) and Anthony Skjellum created a new FPGA testbed and updated the existing IBM Power9 testbed with new nodes.
- In FY2019, 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. Deployment of these resources began in FY2020.

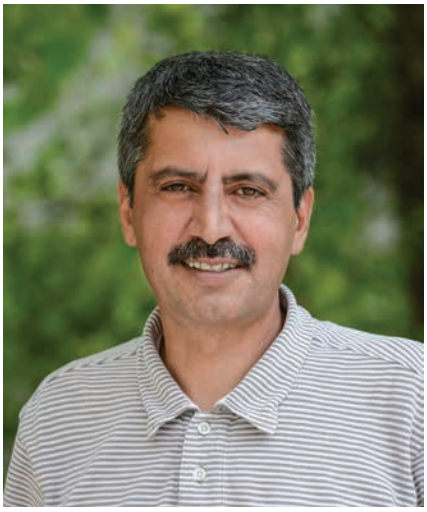
In collaboration, SimCenter, and the Office of the Vice Chancellor for Research continue to foster a rapidly expanding and enhancing culture of securing external funding as an outcome of seed research funding provided by CEACSE. We recognize the challenges for faculty to excel in attracting extramural 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.

FY2020 awardees

- Fernando Alda: "Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)"
- Stephanie DeVries: "A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers"
- Bradley Harris, David Giles, and Chris Dowell: "The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence"
- Loren Hayes: "Using computational approaches to enhance comparative studies of social evolution"Jennifer Hogg, Shellie Acocello, Gary Wilkerson, Yu Liang, and Dalei Wu: "The Use of Augmented Reality–Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"
- Azad Hossain, Mark Schorr, and Jejal Bathi: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"
- Hamdy Ibrahim and Mohammad Mahtabi: "Corrosion modeling of magnesium-based fixation hardware for mandibular reconstruction surgeries"
- Farah Kandah and Mina Sartipi: "Decentralized and Scalable Trust Management Approach via Blockchain for Connected Vehicles in Smart Cities"
- Francesca Leasi, Jejal Bathi, Lani Gao, and Hong Qin: "Simulating bio-environmental interactions using –omics approaches"
- Ashley Manning-Berg: "Modeling of microbial mat decay and implications for the early Earth fossil record"
- Eleni Panagiotou, Jin Wang, Wang-Yong Yang, Chris Dowell, and Abi Arabshahi: "A study on the local and global effects of polymer entanglement in material properties and biological functions"
- Jared Pienkos: "Alkynyl tetrafluoro-pyridyl ligands: computational studies, synthesis, and characterization"
- Reetesh Ranjan: "A multi-fidelity computational modeling strategy for large-eddy simulation of turbulent combustion"
- Sungwoo Yang: "Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling"

SIMCENTER-FUNDED COVID-19 RESEARCH

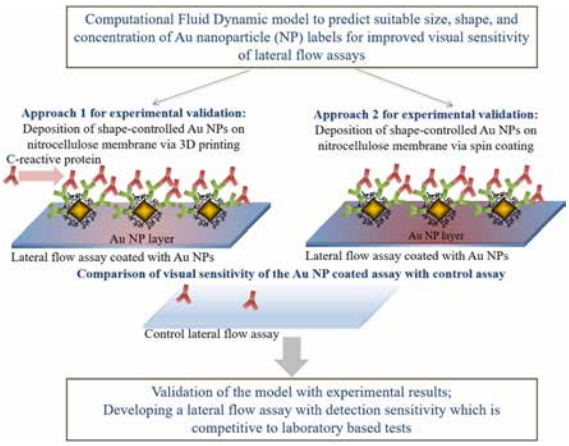
In the early months of the COVID-19 pandemic, the SimCenter prioritized research projects whose goals directly related to detection, mitigation, and treatment of the virus and related infections. CEACSE funds were dedicated to the following four projects that span three engineering disciplines and applied mathematics.



Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles

PI: Dr. Soubantika Palchoudhury, Chemical Engineering; co-PI: Dr. Abi Arabshahi, SimCenter

Testing for COVID-19 requires cost-effective point-of-care (POC) detection assays, which offer non-invasive and rapid diagnostics in a non-laboratory environment, beneficial for rural and low-income areas. Key requirements in engineering a POC diagnostic technique is that it should be simple to use, robust in storage and operation, portable, inexpensive, and able to provide results similar to established laboratory methods. A huge impediment to the success of POC diagnostics is limited detection sensitivity when compared with conventional laboratory methods. For example, lateral flow immunoassay (LFAs), a widely used POC diagnostic technique, is currently 1000-fold lower in analytical sensitivity than comparable laboratory methods. The focus of this proposal will be to develop a new LFA technique with improved sensitivity and reliable detection results, competitive to current laboratory capabilities. This research will answer a fundamental question in POC diagnostics of how to improve analytic sensitivity of the methods through a combined computational and experimental approach to developing and testing a gold-nanoparticle-coated LFA. The new model and POC assay could be incorporated into smart devices (e.g., mobile phone), providing a revolutionary breakthrough in disease response.



A Topological Analysis of Viral Glycoproteins: Application to the Spike Protein of SARS-CoV-2 (COVID-19)

PI: Dr. Eleni Panagiotou, Mathematics

The viral life cycle involves several activities: adsorption, entry, uncoating, transcription, synthesis of viral components, virion assembly, and release. In this research the first two stages are studied, which might be characterized as binding with the host cell and subsequent penetration of the cell membrane. These stages are typically accompanied by a dramatic reconfiguration to create characteristic sequences for binding. Viral therapeutics could be created by disrupting the glycoprotein's ability to recognize its receptor or the ability to rearrange its 3-dimensional conformation. Our goal is to use topology to propose binder molecules to the Spike protein of SARS-CoV-2 that would disrupt its function. More precisely, we propose to use topology to (1) predict residues of high conformational activity from a 3D structure and (2) to combine chemistry, topology, and geometry to quantify the binding affinity of small molecules to the receptor binding domain of glycoproteins. The proposed research provides a particularly innovative approach to both understanding fundamental mechanisms of viral infections and discovering therapeutics. This work is also timely since the scientific community has widely shown that the 3-dimensional conformation of these proteins plays an important role, but rigorous mathematical methods to study them, even for classification purposes, are limited.

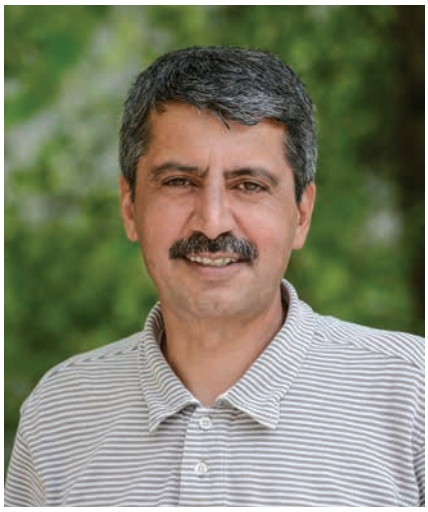
SARS-CoV-2 Nucleoprotein Protein Targeting for Enhanced Covid-19 Theranostics

PI: Dr. Michael Danquah, Chemical Engineering

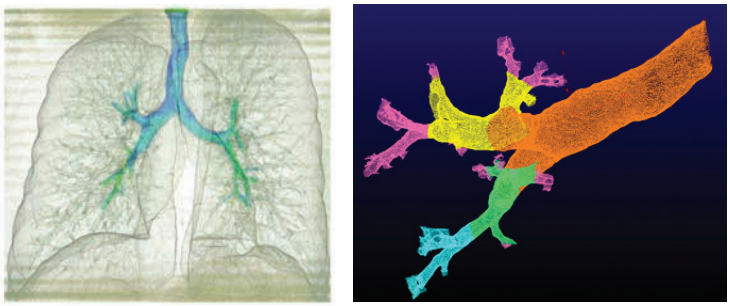
Coronaviruses (CoVs) such as SARS-CoV-2 possess a replicating RNA genome, which makes them good candidates for RNA-targeted diagnostics. Of the four structural proteins of the SARS-CoV-2 virus (S, N, E, and M), targeting the N protein is highly beneficial for SARS-CoV-2 theranostics (a portmanteau of therapeutics and diagnostics) development: it plays a key role in protecting the viral genome and its replication, the viral host infection process, and alteration of the host's immune response. Recently, a SARS-CoV-2 detection technique using a lateral flow assay targeting the N proteins of the virus has been developed; the result was obtained in 30 minutes, representing one of the fastest CoV detection methods to date. This project will build on these results to investigate the molecular mechanisms governing transformations in the structures and binding motifs of RNA aptamers (short RNA molecules that bind to specific target molecules). Structural modeling and molecular dynamics (MD) simulations will target the RNA-binding domains of the N protein to offer real-time analysis and visualization of the aptamer binding process—which will be critical in determining optimal conditions for improved SARS-CoV-2 targeting. The findings from this project will provide significant insights into the binding behavior of the RNA-binding aptamer for enhanced SARS-CoV-2 targeting to improve diagnostics and treatment.

COVID-19-Relevant Computational Modeling of Human Respiratory Airways

PI: Dr. Abi Arabshahi, SimCenter



Complications from COVID-19 can lead to severe pneumonia and pneumonia-like symptoms, including a dangerous and potentially fatal condition known as acute lung injury (ALI) or acute respiratory distress syndrome (ARDS), which is characterized by air spaces becoming filled with fluid. Optimizing aerosolized treatments for a patient in these circumstances requires knowledge of the airflow patterns of the individual's lungs. This project seeks to optimize a computational modeling and simulation process that analyzes CT scans and provides information to healthcare workers of the following variety: (1) detailed information on the structure and characteristics of airflow in the implicated lung(s) and (2) an indication of how much, when, and where an aerosolized drug will transport into diseased/inflamed lungs. These results will be provided as raw outcomes but also reduced into understandable terms for a medical professional through consultation with medical experts in pulmonology. The outcome of this work will be a viable online simulation tool that can, from CT scans of actual patients, provide an analysis of an individual's lung function in 24-48 hours. Currently, the simulation is a long-running process, perhaps as much as a week on a small cluster. This new effort will refine and speed up the process so the results of the simulation can be used to improve patient outcomes early, while they are in the hospital or ill at home.



Simulation of flow within a realistic human respiratory airway. Left: Velocity distribution of particles in the lungs, superimposed on a CT scan; Right: computational mesh visualization of the airways

CENTER FOR UNDERSTANDABLE, PERFORMANT EXASCALE COMMUNICATION SYSTEMS (CUP-ECS)

The SimCenter has been awarded the designation of "PSAAP III Focused Investigative Center" under the banner of the Center for Understandable Performant Exascale Communication Systems (CUP-ECS). The center, led by the University of New Mexico (UNM) in partnership with UTC and the University of Alabama at Birmingham (UAB), is funded by the third iteration of the Predictive Science Academic Alliance Program (PSAAP-III) under the National Nuclear Security Administration (NNSA). The PSAAP III program is a highly competitive group of universities including MIT, UIUC, UT Austin, and Stanford, as well as other household names among the most elite institutions of higher learning in the United States.

Three UTC faculty will co-lead the five-year project: Dr. Tony Skjellum (SimCenter), Dr. Craig Tanis (Computer Science & Engineering), and Dr. Abi Arabshahi (SimCenter). CUP-ECS is poised to create and maintain crucial collaborations with NNSA lab personnel via student exchanges. UTC students--ranging from undergrads to PhD—will undertake R&D working with UTC faculty members and laboratory personnel on some of the most demanding high-performance applications on some of the world's fastest computers. The team will also integrate the center's research into computer science courses at each institution.

Housed across all three universities, center personnel will design, develop, and optimize new communication abstractions, model their performance, and perform roofline-style constraint analyses of their impact on NNSA application performance. These innovations and insights will then be used to help NNSA application and runtime designers understand, predict, and optimize key trade-offs between application communication strategies and application performance. Systematically assessing the impact of these insights on NNSA applications will then lead to yet newer runtime abstractions and optimizations that further improve application performance, resulting in the next iteration of models, assessment, and innovation.

MPI is still the predominant communication system on upcoming exascale supercomputers, and CUP-ECS is specifically looking to develop new abstractions, models, designs, and implementations to revolutionize the development of both MPI and other similar high-end communication systems (e.g. GASNet, Sandia Portals, and others). This work will include developing high-fidelity mathematical models of communication systems to make them faster, easier to understand, and more predictable.

CUP-ECS is also poised to create and maintain crucial collaborations with NNSA lab personnel. These collaborations will be supported by (1) 10-week student visits to the national laboratories (generally during the summer), (2) periodic week-long PI and staff visits to NNSA laboratories, (3) annual NNSA visits to the center, and (4) tutorials and symposia offered by CUP-ECS personnel at conferences and regular laboratory visits.

The team will integrate research, enabling technologies, and application evaluations into multiple courses, teaching core parallel computing techniques to a broad range of students at each institution. At the introductory undergraduate level, students will be introduced to modern parallel computing and communication system concepts. Advanced undergraduate and graduate electives will focus on teaching CUP-ECS-developed techniques in the design of modern HPC applications. Finally, specialized graduate-level electives (potentially also offered as online short courses for NNSA personnel) will focus on mastery of new communication abstractions and models. The courses at each level are as follows:

- Broad Undergraduate: UTC CPSC 2800 Introduction to Operating Systems and CPSC 4550 Computer Networks
- Undergraduate/Graduate Elective: UTC CPSC 5260 Introduction to Parallel Algorithms
- Specialized Graduate: UTC CPSC 7110 High-Performance Scientific Computing

The team will pursue a three-pronged strategy to recruit U.S. students for the Ph.D. degree and postdoctoral programs at each university so that students trained on the projects become strong candidates for further integration into the future NNSA workforce, as follows.

- Recruitment: Offer competitive support to undergraduates in strong U.S. institutions with the potential for exciting Ph.D. topics in HPC, particularly women and ethnic minorities in their respective states and nearby via face-to-face recruitment efforts
- Retention: Provide significant mentoring, support, and guidance to ensure that students and postdoctoral fellows make timely progress, with frequent interaction with nearby national labs for senior students and postdocs providing career development opportunities not as readily available as at other institutions
- Engagement: Connect students and postdocs with laboratory collaborators for internships and/or visits and provide opportunities to attend major conferences during their PhD or postdoctoral program

The research team has a long history of using these techniques to recruit, mentor, graduate, and place U.S. citizens in NNSA/DOE laboratories. The center's PIs have already demonstrated that a research assistantship–to–laboratory internship graduate student pathway improves recruitment and retention of U.S. citizen student researchers.

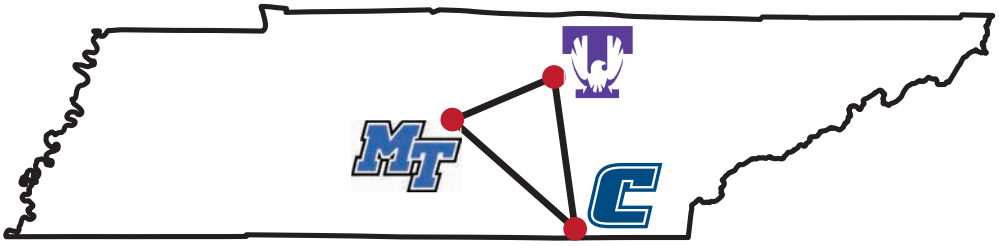
MIDDLE TENNESSEE CYBERINFRASTRUCTURE ALIGNMENT CONSORTIUM (MTCAC)

A team of investigators at the SimCenter, Tennessee Technological University (TnTech), and Middle Tennessee State University (MTSU) have received funding from the National Science Foundation (NSF) for an 18-month Campus Cyberinfrastructure (CC*) project under the cyberinfrastructure research alignment (CRIA) emphasis area. The project's goal is to build a regional consortium to advance collaborative computing research in Middle Tennessee, an underserved but growing area of the nation that combines rural, suburban, and urban areas, and sits at a nexus of major transportation routes and commerce in the Southeastern United States.

Big data and computing are essential to scientific inquiry in the 21st century, and UTC has already demonstrated need for additional resources by securing CC* Networking and CC* Compute awards in 2019. UTC now plans to leverage the local CI improvements that result from these awards to further the networking capabilities of TnTech, MTSU, and other regional institutions via a formalized consortium. This consortium—tentatively to be named the Middle Tennessee Cyberinfrastructure Alignment Consortium (MTCAC)—will help the team enhance our technical collaborations, exchange people and infrastructure with our future partners and one another, and build a larger team to secure additional funding and cyberinfrastructure (CI).

The core project team will pursue the following goals for the Middle Tennessee region:

- Enhance research collaborations between UTC, TnTech, and MTSU
- Assemble a consortium of universities in Middle Tennessee to increase regional networking capabilities and research collaborations



- Improve regional workforce development opportunities
- Develop and implement an innovative plan to broaden participation in computing at consortium institutions and in the surrounding region
- Build proposal teams focused on pursuing external funding to support and expand all other goals

UTC, TnTech, and MTSU have complementary strengths that will only be further complemented by the addition of consortium partners. MTSU, for example, has a strong agriculture component to their research endeavors, and UTC is the strongest of the three team institutions in computational science. Two-year institutions, of which we will recruit at least one, will also have different perspectives on how to integrate improved networking capabilities with their research and education priorities. Proposal teams will focus on additional CC* awards and other NSF programs, including multidisciplinary efforts.

This complementary expertise will advance the research, workforce, and diversity efforts in the region, which will have a great impact on the community, researchers, and students. A major goal of MTCAC is to intensively study approaches to broadening participation in computer/computational science in order to develop and implement a regional plan to recruit and retain students from underrepresented groups. Recruiting minority-serving institutions as consortium members will be a crucial first step. The team is also committed to improving regional workforce development, which will have a broader impact on the students within the teaming institutes and the region. Strong attention to sustainability and ongoing outcomes between and among partner institutions of the consortium will lead to ongoing benefits to faculty and students across the member campuses.

Through the early efforts of this collaboration, the three institutions submitted a proposal to the NSF Research Experiences for Teachers program. The proposed project will offer ten high school computer science teachers from local rural school districts the opportunity to spend ten weeks working with research faculty at UTC, MTSU, or TnTech (whichever is closer to them). During these ten weeks, participants will get hands-on experience with real-world data science, cybersecurity, and high-performance computing projects; engage in regular professional development sessions designed to learn methods of teaching computational thinking to students; and develop curricular modules that integrate the summer research experiences into classroom activities. One major deliverable of the project will be a repository of these modules, freely available to any teacher who visits the repository. Modules will also be directly based on the State of Tennessee educational standards, ensuring optimal integration into existing curricula and increasing the reach of the materials beyond the districts directly impacted by the project.

NEW RESEARCH THRUSTS IN FY2020

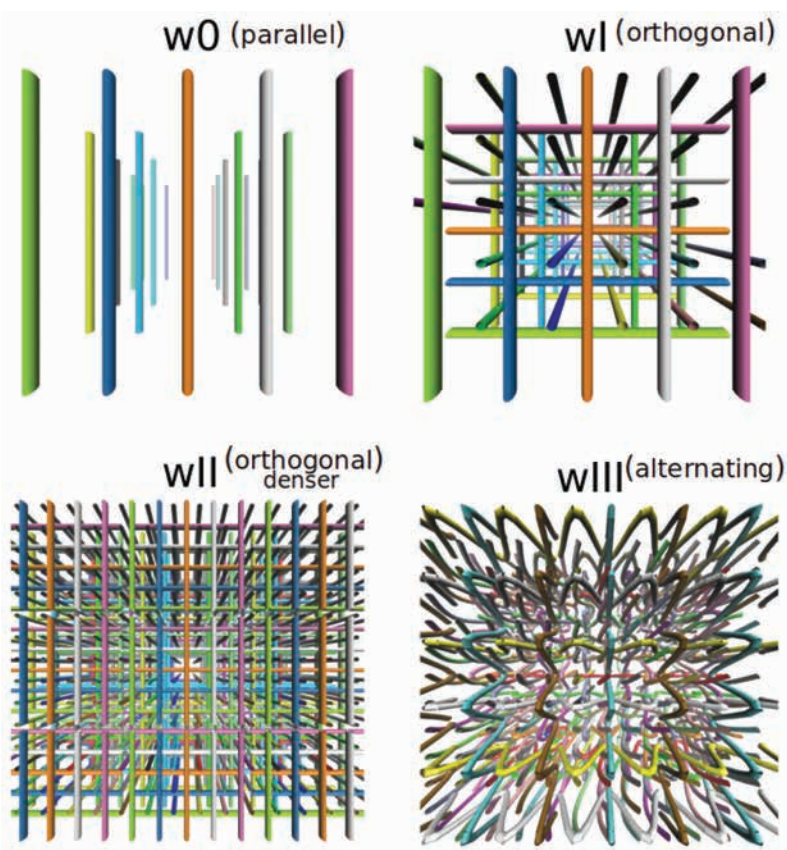
ADVANCED MODELING AND SIMULATION

The Advanced Modeling and Simulation (AMS) research thrust has emerged to fill the gap left by the graduated Aerospace and Defense thrust. Led by Dr. Eleni Panagiotou in Mathematics, this interdisciplinary thrust encompasses projects in bioengineering, living matter, and soft matter. The goal is to create a research program that will be home to a scientific and engineering community that creates new collective knowledge and fosters the next generation of scientific leaders. Other examples of research areas are fluid structure interactions simulations, molecular dynamics simulations, field theoretic simulations, statistical analysis, mathematical optimization, computational fluid dynamics, machine learning, and topological data analysis.

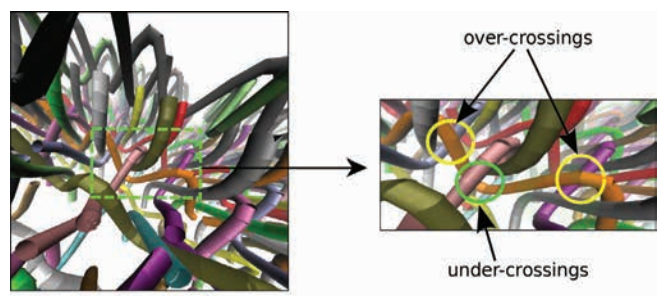
Dr. Panagiotou plans to expand AMS collaborations to industry (Volkswagen, Kordsa Global, Nippon Paint) and national lab partners. Within UTC, she is exploring opportunities to work alongside the Center for Urban Informatics and Progress, the Digital Twins thrust in the SimCenter, and the Health & Biological Systems thrust in the SimCenter. Graduate courses will also be created from the thrust members' research efforts: Applied Knot Theory, Topological Data Analysis, Field Theoretic Simulations, and Simulations of Liquids.

Ongoing projects:

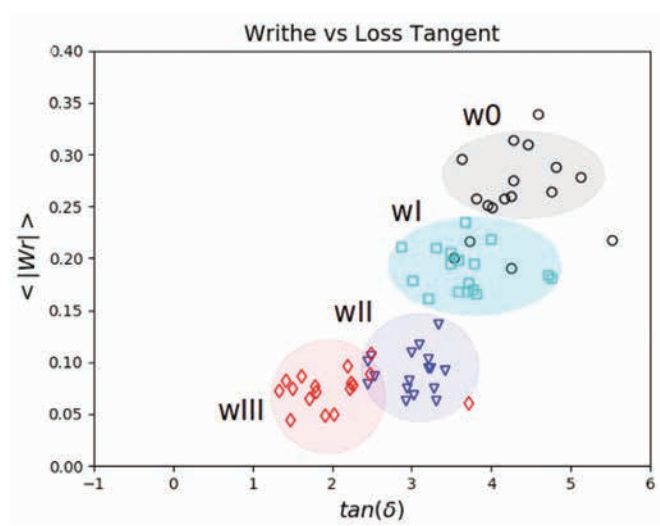
- Creation of topologically optimal metal porous material for medical applications (experimental data and simulation) -- Dr. Panagiotou & Dr. Hamdy Ibrahim (Mechanical Engineering)
- Topology of the mitotic spindle and cell division (experimental data analysis) -- Dr. Panagiotou & collaborators at the University of North Carolina at Chapel Hill and the University of Virginia Medical School
- A topological model for protein folding kinetics (experimental data and simulation) -- Dr. Panagiotou & collaborators at the University of California, Santa Barbara and Princeton University
- Selective sequence Protein Binding (Simulation and experiment) -- Dr. Panagiotou, Dr. Wang-Yong Yang (Chemistry), Dr. Michael Danquah (Chemical Engineering), & Dr. Jared Pienkos(Chemistry)
- Multi-scale modeling of polymers (simulation and experimental data) -- Dr. Panagiotou, Dr. Jin Wang (Mathematics), & Dr. Kumar Rajeev (ORNL)



Weave Topologies



Entanglement of the Polymer Chains



EXTREME ENVIRONMENT TECHNOLOGIES

The Extreme Environment Technologies (ExTReME: **EX**treme environment **T**echnologies and **RE**liable **M**achines and **E**lectronics) research thrust was created in 2019 by Dr. Daniel Loveless (Electrical Engineering). Extreme environment electronics and computing systems represent a vital niche industry within the trillion-dollar global electronics infrastructure. The field involves the design and implementation of semiconductor devices, circuits, subsystems, and systems capable of operating within environments outside of typical commercial domains. Examples include operation in radiation-rich, low-temperature, high-temperature, wide-temperature range, vibrationally intense, chemically corrosive, or magnetically intense environments. Further, operation under combined extreme conditions is quite common and can be readily observed in many space missions.

Microelectronics technologies' unwavering progress has resulted in technologies that are predictably more advanced with each coming year. Advancement occurs through so-called Moore's Law scaling, as well as the occasional disruption. With the continued improvement of microelectronics, the fields within extreme environment systems have seen increased vulnerabilities and uncertainty in performance with each disruption. The Extreme Environment Technologies thrust aims to tackle some of the preeminent challenges faced by the use of the most innovative technologies in extreme environments, thus enabling reliable, high performance computing for the advancement of science.

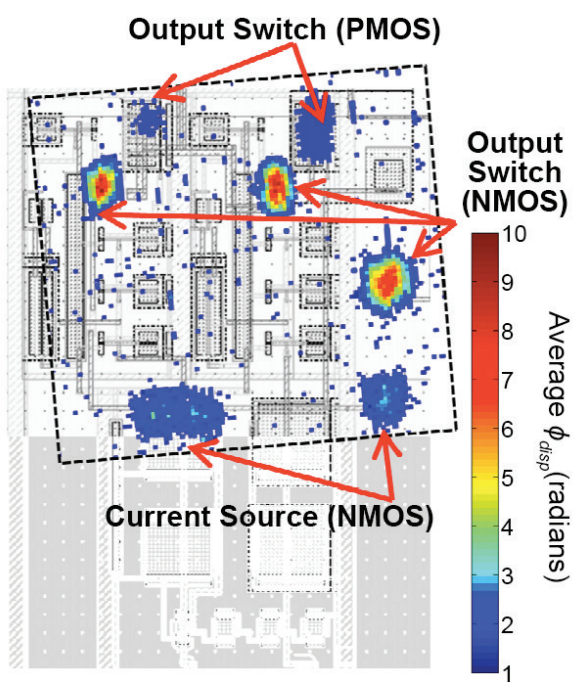
Mission

- Enable students to research emerging technological problems related to the space sciences and high-reliability electronics
- Provide solutions to some of the most challenging problems faced by future electronics systems
- Encourage continued study and practice in STEM fields
- Broaden participation in the space sciences.

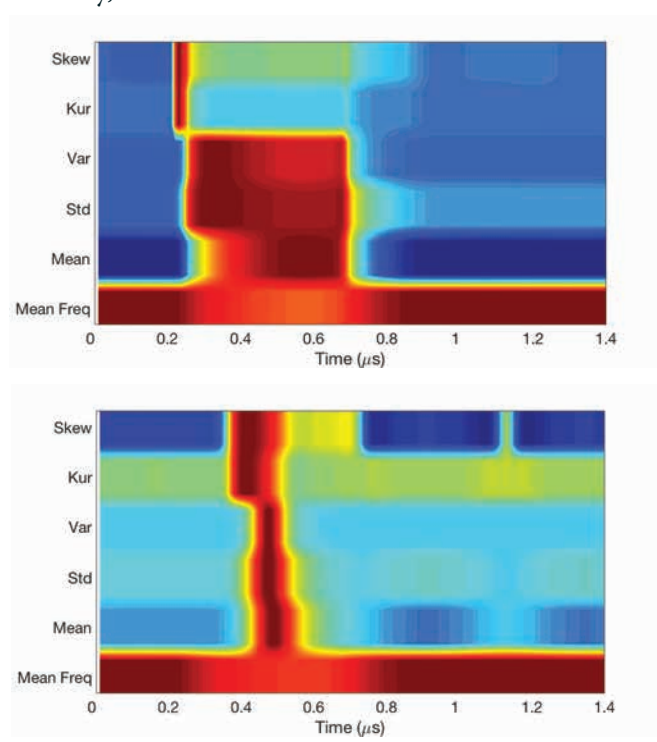
Research areas

- Earth and Space Exploration Systems
- Electronics radiation effects
- Reliability
- Trust
- Systems-of-systems
- Additive manufacturing
- Automotive electronics

Ongoing projects are funded by the Defense Threat Reduction Agency (DTRA), the U.S. Army, the National Science Foundation (NSF), and the Air Force Research Laboratory (AFRL). These projects leverage partnerships with universities, government agencies, national labs, and for-profit companies. Examples include the Missile Defense Agency, NASA GSFC, Scientic, Nu-Trek, Purdue University, Vanderbilt University, Arizona State University, Georgia Tech, Brigham Young University, and AFIT.



A two-dimensional (2D) spatial map of the regions within an integrated circuit that are sensitive to radiation-induced transient anomalies. Data were captured at the Naval Research Laboratory.



Example IRES spectral images showing statistical properties of the radiation-induced transient anomalies. The statistical properties are used for training machine-learning algorithms for automated identification of the faults.

REVV! (TENNESSEE MANUFACTURING INNOVATION PROGRAM)

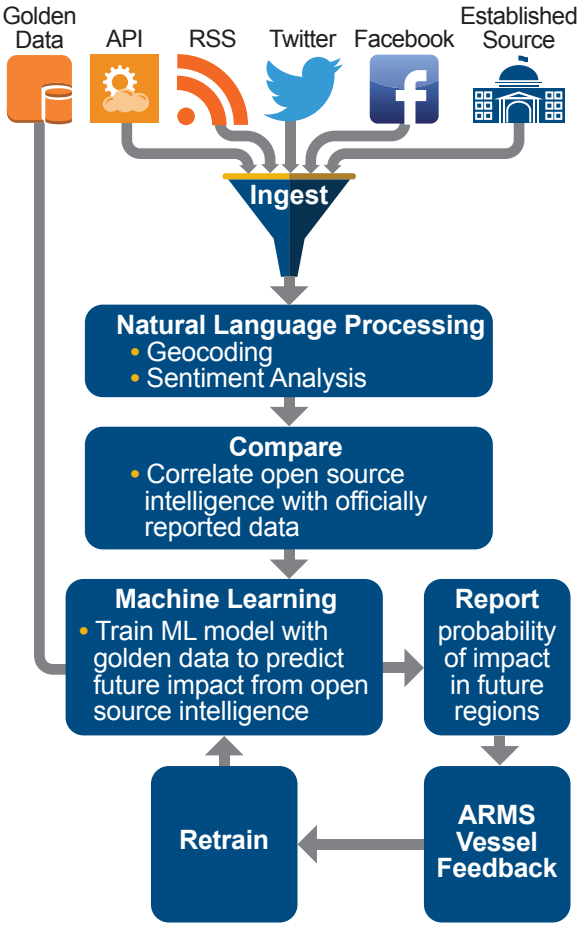
In FY2020, the SimCenter was involved with two projects from the RevV! program, part of a $2.5 million manufacturing innovation program created by the State of Tennessee in partnership with the University of Tennessee and Oak Ridge National Lab (ORNL). RevV! allows the winning manufacturers, product developers, and researchers access to state-of-the-art computing and other facilities at ORNL, in addition to up to $250,000 in funding. One project began in FY2019 and will be completed in FY2021; the second was funded at the end of FY2020 and will begin in FY2021.

International Maritime Security Associates (IMSA)

In FY2020, SimCenter faculty collaborated with IMSA on a project funded by RevV!. IMSA is a small, veteran-owned business whose 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. IMSA is helmed by Corey Ranslem, with operations centers in South Florida, Chattanooga, and London.

IMSA
International Maritime Security Associates

The goal of this collaboration was for SimCenter personnel, including Dr. Don Reising (UTC Electrical Engineering), Dr. Farah Kandah (UT Computer Science & Engineering), Dr. Skjellum, and their 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, allowed IMSA to complement their existing data-gathering infrastructure. The Global Intelligence, Information and Communications Center (G-I2C) maintains a carefully maintained source of information and intelligence available 24/7 to supported mariners anywhere in the world.



The project, to end in December 2020, has so far emphasized research on connecting a particular phrase found in social media and other text feeds to a geographic location. The motivation behind the correlation originally was to determine possible maritime risks for ships in a certain area. The locations would then be compared to a list of ports, World Port Index. If a port matched a location, the algorithm would search that area for the particular phrase and return the results (Tweets or Feed Posts). This portion of the work has been completed successfully, with several rounds of iteration.

The next phase of the project focused on improvements to the base system. Jacob Coleman, IMSA Director of Information Technology, chose a new core software that allowed him to identify some new areas of analysis, including determining a level of importance or priority. In addition, the team added a simple source identifier (Twitter, RSS, JSON) to break locations down by source. Another significant enhancement involved improving the reliability of the communications link between vessels and the data center. Dr. Reising and his student, Ahmed Ibrahim, used random linear network coding (RLNC) to encode data for faster transfer with reduced data loss.

The remaining goals for the project are to compile and test an initial database setup, move to large-scale testing, and connect continuous sources and multiprocessing for more efficient data analysis.

Hayden Data Systems

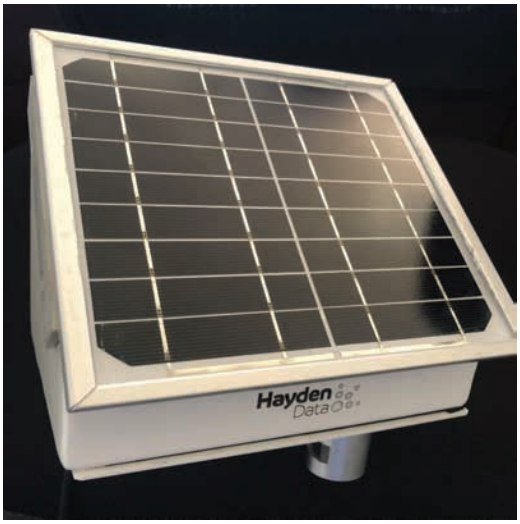
At the end of the fiscal year, Dr. Don Reising partnered with Hayden Data Systems, an emerging technology organization whose strategy is to leverage the growing market for Internet of Things (IoT) sensor technologies. Hayden Data Systems is a Tennessee-based organization located in Chattanooga with offices and facilities in Colorado and Australia. They combine IoT sensors with advanced analytical tools including Artificial Intelligence (AI) and Machine Learning (ML) to create efficient and effective outcomes for organizations and communities.

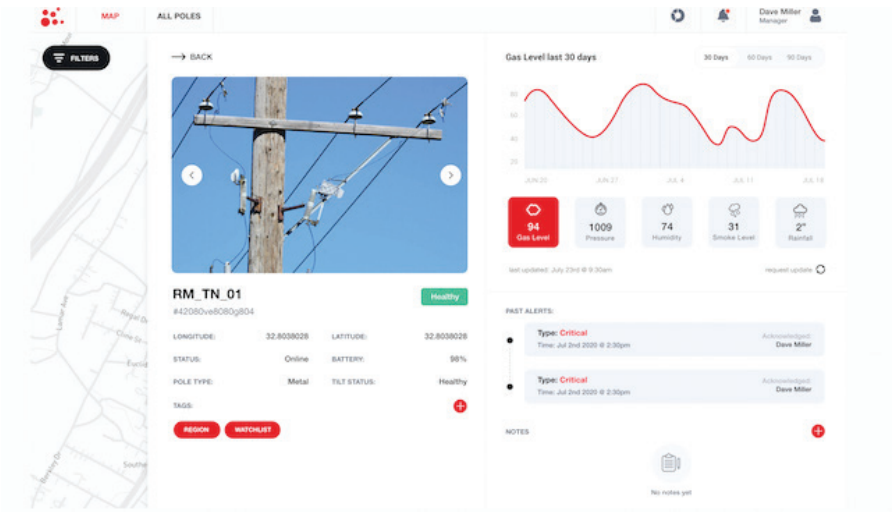
The company's vision is to deliver actionable information to their customers enabling them to make critical decisions effectively; provide situational awareness to deliver a conceptual understanding of what is or will affect communities, assets, and organizations; and deliver clear and concise knowledge of all the elements that will impact them.

Hayden Data Systems' Safe Power Network (SPN) technology provides an asset condition monitoring information service to the electric power industry for their power pole population. Distribution power poles are often considered low priority because of their longevity (50+ years) and are inspected using a rotational process; thus, pole health and nearby vegetation are not monitored routinely. Consequently, pole failures can occur undetected and result in power interruptions and fires. With SPN instruments monitoring each pole, taking measurements every five minutes, and capturing an overhead camera image every 3-6 months for vegetation management, actionable management information is provided before failures occur.

To enhance SPN, further research and development are required. This RevV! project proposes three needed enhancements to the monitoring system: energy harvesting, alternative energy storage, and current monitoring. Energy harvesting and storage enhancements will allow battery recharging under low-light and extreme winter weather conditions, due mainly to lack of sunlight (heavy clouds or snow coverage). Additionally, devices installed in these extreme winter or mountainous regions require an on-board heater to ensure reliable communication of sensor data. This heater requires power beyond what the present solar-powered device can provide. Finally, information on current transmitted through each conductor is required to complete algorithms for predicting pole strength. Because of the lack of current measurement devices, R&D of a wireless current transformer is required so these devices can provide real-time data for each conductor of each distribution network branch.

This project will lead an enhanced SPN solution that will then lead to additional revenue and customers by growing Hayden Data Systems' market share within Tennessee, the southeast, the United States, and ultimately the world. The development and eventual production of this next-generation SPN will lead to the following over the next five years: (1) the creation of 55 Tennessee jobs, (2) a minimum $5 million capital investment in Tennessee, and (3) a projected annual revenue of $9 million.





STUDENT PROFILES

GRACE NANSAMBA I completed a Bachelor's degree in Information Technology from Makerere University, Uganda in 2015. I am working toward a Master's degree in Computer Science at UTC, graduating in fall 2020.

My MS thesis work involves the second-generation poly-algorithm library, with the aim of optimizing performance of parallel, dense linear algebra libraries. I am varying the algorithm as a function of problem, concurrency, and architecture, with new additions compared to the prior work. This is an advancement on the poly-algorithm library that was designed in 1993 and has several generalized parallel dense matrix multiplication algorithms of the form C = AB + C on two-dimensional process grids. The advances in computers over the past 25 years since this work was done makes it meaningful to review and re-tune these algorithms, as well as to extend them based on other work done in the meantime. A new intra-node BLAS kernel that was designed to improve performance of the DGEMM in fat-by-thin dense matrix multiplication, which often occurs as generic sub-problems inside parallel dense matrix multiplication, was integrated. A modern parallel SUMMA algorithm that is rank-k based was added, which increases the opportunity for parallelism compared to the rank-1 based SUMMA incorporated in the original library.

To get the results for this work, I carried out simulations on the SimCenter computer clusters, the Tennessine or OneSeventeen, and I am still running some more. I had assistance from SimCenter faculty and students to complete my runs successfully, and we had in-depth discussions to understand the results and draw conclusions.

I have an awesome group of students who are collaborating with me to learn more about high-performance computing for linear algebra libraries, debug code, and explore performance of parallel systems. Some of these students are from Tennessee Technological University and together we have spent countless hours running simulations on SimCenter machines and on Stampede2 supercomputers from TACC at the University of Texas at Austin.

I am starting my PhD in Computational Science: Computer Science at UTC in spring 2021. I currently work with Dr. Skjellum and will continue with him for my PhD. My work will be in the area of exascale computing systems, parallel programming, and performance understandability.

SEVAUGHN ORR My educational background is in computer science, math, and psychology. I am working toward a BS in Computer Science: Software Systems, with a minor in Psychology. I currently work for Dr. Skjellum and Dr. Kandah, focusing on applications of machine learning to cybersecurity.

In summer 2019, I interned at EPB with the network team, where I helped with managing the data center and servicing network issues. I also travelled to various workspaces throughout Chattanooga to service network-related issues. One project I worked on involved automating weather advisory signals for weather events. I achieved this work using Python to query ArcGIS endpoints for weather data. The application then analyzed signals such as storm area, pressure, meteorologist warnings, etc. After analysis, the application sent an update to the content management system to notify analysts.

In January 2020, I began my internship with the Tennessee Valley Authority where I currently work in Pricing & Contracts performing data transformation, visualization, and analytics. At TVA, one of the projects I work on is a wholesale energy pricing study. In this project, we generate hypothetical scenarios to analyze the impacts of changes to wholesale energy rates. Analyses are conducted by reviewing visuals developed in Microsoft's PowerBI and through decision modeling using the analytic hierarchy process. Before transitioning to research at the SimCenter, I assisted the System Administrator servicing user tickets. One of the projects I worked on was the upgrade of the legacy hadoop clusters. This process was done by building an Ansible automation script to perform tasks outlined in documentation created by the opensource organization openHPC.

After graduation, I hope to remain in Tennessee or a bordering state; however, I am open to going wherever the best opportunity is for me. I know that if I continue to intern with TVA there is a strong chance a full-time position will come of it. After being in the workforce for a while. I think it would be nice to return to school and pursue a master's degree.

STUDENT PROFILES

TOM HERSCHBERG I am a rising senior finishing a BS in Computer Science with a focus in cybersecurity. I am currently working on two projects at the SimCenter: one with Dr. Tony Skjellum and one with Dr. Eleni Panagiotou.

This summer, I began an internship with Los Alamos National Laboratory in Los Alamos, New Mexico, which I will be continuing during the upcoming academic year. My work there involves helping prepare the current Open-MPI Sessions prototype for integration back into the main code base. Specifically, I spent this summer extending the prototype to be compatible with the network stack (OFI Libfabric) that is expected to be included in many exascale systems. In the fall, I will focus on rigorously testing the Sessions prototype in preparation for its eventual inclusion in the main Open-MPI code.

My main research focuses for FY2020 were high-performance computing and applied knot theory. I worked with Dr. Skjellum on adding MPI Sessions functionalities to ExaMPI, a research-oriented MPI implementation. We are now using ExaMPI to develop applications and use cases for MPI Sessions, as well as expand MPI Sessions' capabilities. With Dr. Panagiotou, I researched how to extend LAMMPS, a molecular dynamics simulator, to enable the measurement of topological entanglement. We created a package for LAMMPS that uses the Gauss linking integral to measure the entanglement of polymers during a LAMMPS simulation.

My collaborations with Derek Schafer on ExaMPI, Dr. Howard Pritchard on Open-MPI and MPI Sessions, and Dr. Panagiotou on applied knot theory all began in the past year. They were all also set up with the help of Dr. Skjellum, who has been instrumental in my success at the SimCenter. I plan to continue my research with both the SimCenter and LANL this year. I also plan to research how MPI Sessions can be used to simplify the creation and use of topological communicators in MPI.

In FY2021, I will serve as the student representative for the SimCenter Leadership Council. When I complete my MS, I plan to pursue a PhD in Computer Science.

JAPORSCHE PETTAWAY I have a BA from UTC in English (Creative Writing) with a minor in Geology and am currently pursuing an MA in English (Creative Writing). I am the first-ever Editing and Proposal Development Specialist in the SimCenter, working with Bailey Kirby, the Grant Administrator.

My current assistantship role includes proofreading and copy-editing proposals, sanitizing and editing PDFs in addition to sending emails, fashioning award letters, gathering and organizing information, and other duties as required.

Much of my role has so far has involved editing grant proposals and journal manuscripts. I also assist with portions of the CEACSE funding competitions, including proofreading proposals, preparing award letters, and managing a reviewer database. In my second year, I will likely have more proposal and writing duties.

My prior research has included linguistics, race relations, mental health issues, and discrimination against minorities. In addition, I'm interested in critical analysis of film, books, and television. Having experience in both English and Geology really readied me for this role at the SimCenter. Both areas are technical and demanding, with a lot of independence involved. Though my work does not include as much collaboration as more technical research assistantships might, I provide crucial support (editing, proofreading, etc.) to SimCenter faculty and staff. It's not lost on me that I encounter the work of some extraordinarily intelligent people!

I genuinely enjoy editing and proofreading work for quality, so my goal is to snag an Editor-Writer position after (or during) my Master's tenure. In the meantime, I am completing my thesis for Spring 2021. It will probably be a speculative fiction novella or something similar. Eventually, I intend to pursue a PhD in English, Communications, Women and Gender Studies, or even Film Studies.

FUNDED PROPOSALS IN FY2020

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 18 following SimCenter-affiliated proposals were funded in FY2020, for a total of $2,831,749.

Title	PI	Funding Agency	Amount
RUI†: Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems	Dr. Abdollah Arabshahi	NSF	$42,269
Contract: ATSE Spack	Dr. Tony Skjellum	Sandia National Laboratory	$30,000
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	$50,000
Collaborative Proposal: ECR: PEER: Software Engineering Workforce Development in High-Performance Computing for Digital Twins	Dr. Tony Skjellum	NSF	$57,635
REU 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	$16,000
REU Supplement for SHF: Small: Collaborative Research: Coupling Computation and Communication in FPGA-Enhanced Clouds and Clusters	Dr. Tony Skjellum	NSF	$16,000
RUI: Computational Methods for Measuring Topological Entanglement in Polymers	Dr. Eleni Panagiotou	NSF	$125,000
Fault Tolerant MPI Research	Dr. Tony Skjellum	Lawrence Livermore National Laboratory	$60,000
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	$1,406
SPX: Collaborative Research: Intelligent Communication Fabrics to Facilitate Extreme Scale Computing	Dr. Tony Skjellum	NSF	$450,097
Contract: Partitioned Communication Project	Dr. Tony Skjellum	Sandia National Laboratory	$100,000
Fundamental Research into Radiation Effects in Cryogenic Electronic Technologies	Dr. Daniel Loveless	Air Force Research Laboratory	$202,958
Aerostructural Analysis Supporting the Development of Hypersonic Vehicle Flight Test Structures	Dr. James Newman	University of Dayton Research Institute	$737,078
HDR DSC: Collaborative Research: ADACE - Anthropo-centric Data Analysis for Community Enrichment	Dr. Yu Liang	NSF	$723,641
Heterogeneous HPC for High-order Stabilized Finite-elements on Moving and Deforming Domains	Dr. Kidambi Sreenivas	Engility Corporation	$59,799
CC* CRIA: Planning a Regional Cyber-Infrastructure-Research Consortium for Middle Tennessee	Dr. Tony Skjellum	NSF	$249,713
RUI: Computational Methods for Measuring Topological Entanglement in Polymers	Dr. Eleni Panagiotou	NSF	$125,000

† *Research in Undergraduate Institutions (RUI)*

SELECTED FY2020 PUBLICATIONS AND PRESENTATIONS

CONFERENCE PRESENTATIONS, POSTERS, AND PROCEEDINGS

Hossain, A., and Blanton, R., 2019, Quantitative Estimation of Surface Water Quality Parameters Using Remote Sensing Technology in Southeast Tennessee. Chattanooga Development Symposium, August 6, 2019.

Hossain, A., Blanton, R., and Mathias, C., 2019, Quantitative Remote Sensing of Surface Water Quality in Southeast Tennessee. AGU Fall Meeting, 9-13 December 2019, San Francisco, CA.

Roy., S., Atolagbe., B., Ghasemi., A., **Bathi., J. R.** "A MATLAB-based Grid Generation Tool for Hydrodynamic Modeling" ASCE Environmental and Water Resource Institute (EWRI) Conference, Henderson, NV, May 17 – 21, 2020.

Preyanka Dey, **Jejal Reddy Bathi, Francesca Leasi** "Hydrologic models to evaluate pollutant's impacts on microbiology", Tennessee Water Resource Symposium, Montgomery Bell State Park, Burns, TN, April 22 – 24, 2020.

Preyanka Dey, **Jejal Reddy Bathi, Francesca Leasi** "Hydrological Modeling of South Chickamauga Creek watershed using BASINS/HSPF", TNSA Annual Conference Going the Distance in 2020. (Podium presentation)

Hossain, A., Blanton, R., and Mathias, C., 2019, 2020, Quantitative Remote Sensing of Surface Water Quality in Southeast Tennessee Utilizing Planet Dove Imagery, 69th Annual Southeastern / 55th Annual Northeastern Section Meeting – 2020, 20-22 March 2020, Reston, Virginia (Abstract accepted). Conference canceled due to COVID-19 situation.

Panagiotou, E., International Symposium, Polymers and networks, Ochanomizu University, Tokyo, Japan, August 2019.

Panagiotou, E., Program on Biological Physics of Chromosomes, KITP, June-July 2020 (virtual)

Panagiotou, E., Women in Mathematics of Materials, Association of Women in Mathematics, SIAM, July 2020 (virtual)

J. Wang, "Immersed boundary and immersed domain methods for fluid-structure interaction", Special Session on Applicable Analysis and Control Theory for Fluid and Fluid-Structure PDEs, SIAM

Y. W. Wang, talk at SERMACS 2019, October 2019

Moataz Abdalla, and **Hamdy Ibrahim**. "Corrosion modelling of coated pure magnesium towards degradation-controlled bone fixation implants". Materials Science & Technology 2020, Pittsburgh, PA, USA.

Kandah, F. IEEE High Performance Extreme Computing Conference (HPEC)

Kandah, F. IEEE 9th Annual Computing and Communication Workshop and Conference (CCWC).

Neglia, S.; Lee, J. P.; **Pienkos, J. A.** Synthesis, characterization, and reactivity of a heterobimetallic organometallic complex with a trans bidentate ligand for catalytic carbon-hydrogen bond activation. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Truong, T. T.; Mconkey, A. M.; Moser, Z. D.; McDarmont, S. L.; Lee, J. P.; Wang-Yong, Y.; **Pienkos, J. A.** Synthetic strategies for generating 4-ethynyl-2,3,5,6-tetrafluoropyridine. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Jaques, L. D.; McDarmont, S. L.; McMillen, C.; Neglia, S.; Lee, J. P.; **Pienkos, J. A.** Synthesis of tbpyPt(C22py)2 and its interactions with Cu(I) and Pd(II) metals. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Strike, W., Martin, D., Glass, K., **Harris, B.** Phospholipid remodeling via exogenous polyunsaturated fatty acid uptake modulates stress resistance in Vibrio cholerae. Poster presented at: AIChE National Conference; 2019 November 11; Orlando, FL.

Rojas, E., Giles, D., Wang, J., and **Harris, B.** Influence of population density and environmental conditions on V. cholerae growth and virulence. ASM Microbe 2020 June 18-22; Chicago, IL (abstract accepted for poster presentation, conference postponed).

Turgeson, A., **Harris, B.**Elucidation of the mechanism of long-chain fatty acid recognition in V. cholerae: an in silico study. American Institute of Chemical Engineers Annual Meeting 2020 November 15-20; San Francisco, CA (abstract accepted for conference paper).

Hogg, J., OPTIMAL-Based Virtual Reality Feedback to Reduce Dual-Task Balance Cost, 2020 Virtual Meeting of the American Society of Biomechanics (will be refereed in the Journal of Biomechanics)

Alda, F. 2020 Joint Meeting of Ichthyologists and Herpetologists (cancelled)

DeVries, S. Nitrate Model, Wisconsin Department of Natural Resources. 2020.

Carpenter, **Hayes** and Tanis, presented (via Zoom) the automated search tool to unfunded collaborator Schradin's lab group, IPHC-Strasbourg, France.

R. Ranjan, AIAA SciTech Forum and Exposition, 2020, Orlando, FL, USA.

SOFTWARE

R. Ranjan, AVF-LESLIE: It is a fully compressible flow multi-physics solver, originally developed at GT within the Computational Combustion Laboratory (CCL) directed by Prof. Suresh Menon.

R. Ranjan, OpenFoam: An in-house version of OpenFOAM is being developed and maintained by the PI at UTC to carry out applied research activities.

REFEREED PUBLICATIONS

Bathi., J. R., Roy., S., Computer Tools for Urban Hydrology and Water Quality Management, In Sustainable Water: Resources, Management and Challenges, Nova Science Publishers, Inc, NY, USA, 2020.

Panagiotou E. and Kauffman L. H., 2020, Knot polynomials of open and closed curves Proc. R. Soc. A (accepted)

Panagiotou E. and Plaxco, K. W., 2020, A topological study of protein folding kinetics Topology of Biopolymers, AMS Contemporary Mathematics Series 746

Panagiotou E., Delaney K. T. and Fredrickson G. H., 2019, Theoretical prediction of an isotropic to nematic phase transition in bottlebrush homopolymer melts, J. Chem. Phys. 151, 094901

Abdalla, Moataz, Alexander Joplin, Mohammad Elahinia, and **Hamdy Ibrahim**. "Corrosion Modeling of Magnesium and Its Alloys for Biomedical Applications." Corrosion and Materials Degradation 1, no. 2 (2020): 219-248.

Yang, S. "Thermal and Mechanical Properties of 3-Dimensional Carbon Network as Flexible Thermal Additives" (in progress, 50%).

Yang, S. "Optimization of The Adsorbent Geometries of Water Harvesting System by Finite Element Method" (in progress, 65%).

F. Kandah, B. Huber, A. Altarawneh, S. Medury and A. Skjellum, "BLAST: Blockchain-based Trust Management in Smart Cities and Connected Vehicles Setup," 2019 IEEE High Performance Extreme Computing Conference (HPEC), Waltham, MA, USA, 2019, pp. 1-7, doi: 10.1109/HPEC.2019.8916229.

F. Kandah, A. Altarawneh, B. Huber, A. Skjellum, and S. Medury, "A Human-Understandable, Behavior-based Trust Management Approach for IoT/CPS at Scale," Int. J. of International Society for Computers and Their Applications (ISCA), In Press (2020)

J. Coleman, **F. Kandah** and B. Huber, "Behavioral Model Anomaly Detection in Automatic Identification Systems (AIS)," 2020 10th Annual Computing and Communication Workshop and Conference (CCWC), Las Vegas, NV, USA, 2020, pp. 0481-0487, doi: 10.1109/CCWC47524.2020.9031248.

A. Altarawneh, T. Herschberg, S. Medury, **F. Kandah** and A. Skjellum, "Buterin's Scalability Trilemma viewed through a State-change-based Classification for Common Consensus Algorithms," 2020 10th Annual Computing and Communication Workshop and Conference (CCWC), Las Vegas, NV, USA, 2020, pp. 0727-0736, doi: 10.1109/CCWC47524.2020.9031204.

Jaques, L. D.; McDarmont, S. L.; Smart, M. M.; McMillen, C. D.; Neglia, S. E.; Lee, J. P.; **Pienkos, J. A.**, Structural characterization of the metalloligand tbpyPt(C22-py)2 and its interaction with Pd(OAc)2. Inorganic Chemistry Communications 2020, 112, 107722. (IF 1.943)

Pienkos, J. A., Exploiting a C-F activation Strategy to Generate Novel Tris(pyrazolyl)methane Ligands (submitted ZAAC, IF 1.24)

Hogg, J., Wellness Survey Responses and Smartphone App Response Efficiency Associate with Remote History of Sport-Related Concussion, Perceptual and Motor Skills (under review)

DeVries, S., Bradbury, K., and Cardiff, M. "A Groundwater Flow Model for Waupaca, WI." Wisconsin Geological Survey and Natural History Survey Technical Report.

R. Ranjan, and S. Menon, "Application of Nonlinear Reduced Order Modeling Strategy for Large Eddy Simulation of Chemically Reacting Turbulent Flows", AIAA-2020-2140, AIAA SciTech Forum and Exposition, 2020. (DOI: https://doi.org/10.2514/6.2020-2140)

R. Ranjan, Assessment of Two Level Simulation Model for Compressible Turbulent Mixing Layer, Accepted, 17th International Workshop on the Physics of Compressible Turbulent Mixing, Atlanta, USA, July 13-17, 2020.

Preyanka Dey, **Jejal Reddy Bathi, Francesca Leasi**, "Sensitivity of HSPF Model watershed hydrology for BASINS 4.5 Land Cover and Meteorological Databases" (manuscript under preparation)

SIMCENTER STAFF

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 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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