THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

Annual Report to the Tennessee Higher Education Commission: Fiscal Year 2017–2018

OCTOBER 24, 2018

Submitted by
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THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

SIMCENTER

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

MISSION STATEMENT

To establish, expand, and sustain a cohesive multidisciplinary effort in applied computational sciences leveraged across UTC to produce sustained growth in research funding, excellence in integrated education and research, growing numbers of Ph.D. graduates in these applied areas, and increased national and international stature and competitiveness in Tennessee.

VISION STATEMENT

UTC's cohesive multidisciplinary effort in applied computational sciences is recognized for its contributions to the community, the state of Tennessee, the region, and the nation for its solution of problems of importance to society, including the creation of useful inventions based on applied science and engineering research. Participating undergraduate and graduate students from UTC graduate to become knowledge workers who, through their specialized training, contribute routinely to their community, state, region, and nation.

EXECUTIVE SUMMARY

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 FY2017, CEACSE marked its twelfth 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 FY2018 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 Ph.D. students.

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

The high-performance computing (HPC) capabilities associated with the recently acquired UTC heterogeneous GPU-enabled cluster (a high-end, 33-node, 64-bit Intel-architecture cluster with NVIDIA P100 GP-GPUs) and a newly acquired 4-node, IBM Power9 cluster with quad-NVIDIA-V100 GPUs were both important differentiators that led to key programmatic accomplishments in FY2018. The addition of a petabyte of DDN storage in December 2017 to replace earlier storage and backup further enabled our researchers in their quantitative and scientific work.

Notable outcomes of FY2018:

- The Smart Cities & Urban Dynamics swim lane[1] graduated into its own research center at UTC: Center for Urban Informatics and Progress (CUIP). This center's inaugural director is Dr. Mina Sartipi, who led the original swim lane and continues to lead campus-wide efforts on Smart Cities and related R&D. Support from CEACSE leveraged

[1] "Swim lane" is our preferred terminology meaning area of emphasis, pillar, or "vertical."

into external support from NSF and others and has now enabled this second academic center to emerge on campus. SimCenter will continue to be a resource to CUIP, and faculty associated with it continue to submit proposals in the modeling and simulation area related to smart cities. More information about CUIP may be found here: http://bit.ly/UTC-CUIP.

- Dr. Don Reising (Electrical and Computer Engineering) has assumed the leadership role for the Energy & the Environment swim lane.
- Dr. Craig Tanis (Computer Science and Engineering) has assumed the leadership role for the new swim lane for HPC.
- Dr. Farah Kandah (Computer Science and Engineering) has assumed the leadership role for the swim lane for Cybersecurity & Cyber-physical Systems.
- We have established research focus groups for Health & Biological Systems as part of the swim lane now led by Dr. Hope Klug (Arts and Sciences), who is now also the Interim Chair of Biology. Two interdisciplinary research tracks are active as of this report: Hospital Health Modeling and Simulation, and Interdisciplinary Math/Computer Science/Biology and Ecology Ideation.
- Dr. Eleni Panagiotou was hired as a new professor of mathematics. Her work in modeling and simulation applies to problems with complex physics and geometry in biological and chemical engineering (e.g., rheology) and many other application areas.

Important technical advancements achieved in FY2018 include these highlights:

- Dr. Robert Webster was funded by Engility Corporation for work on “Heterogeneous HPC for High-order Stabilized Finite-elements on Moving and Deforming Domains.”
- The SimCenter research network infrastructure was updated to support Internet of Things, smart cities prototyping, and cyber/systems activities. This specialized network allows scientists and engineers to work in parallel with the university’s production network while avoiding security concerns. This update is a prelude to supporting a DMZ, data transfer node, and other research infrastructure in FY2019 and beyond.
- Dr. Hong Qin (Computer Science, PI) together with Drs. Hope Klug (Biology), Joey Shaw (Biology), Jennifer Boyd (Biology), and Azad Hossain (Environmental Sciences) received a major National Science Foundation (NSF) Award for Big Data R&D entitled “Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education Award.” This work will be supported by SimCenter as it kicks off in October 2018. Our goal will be to connect Big Data outside UTC with SimCenter infrastructure that will support these faculty members and our Health and Biosystems and Energy and Environment swim lanes. All of the professors involved have received current or prior CEACSE funding support.
- Dr. Abdollah Arabshahi has implemented and validated the third-order MUSCL-type numerical flux formulation scheme and extended to higher-order accurate (up to ninth-order spatial accuracy and second-order temporal accuracy) weighted essentially nonoscillatory (WENO) scheme in the structured flow solver for high-speed flow simulations.
- Dr. Skjellum’s research group, together with collaborators at Clemson University, launched a new blockchain technology based on funding from NSF, keyed to data provenance. This work has direct impact on HPC workflows, and the team has

expanded its scope and incorporated collaborators at the University of South Carolina and the University of Alabama at Birmingham to explore HPC Workflows, reproducibility, and data provenance. Collaborations in this area and in blockchain have commenced with Oak Ridge National Laboratory (ORNL) as a consequence of this R&D work.

- Dr. Skjellum received R&D support from NSF in HPC for the project entitled "Next-Generation Message Passing for Parallel Programming: Resiliency, Time-to-Solution, Performance-Portability, Scalability, and QoS."
- SimCenter received an IBM Award for Machine Learning R&D ($20,000) and regional collaboration in federated clouds.

Additionally, the new IBM Power9 cluster is instrumental in the work of faculty recruited during FY2018 and beyond, including HPC research conducted by Drs. Skjellum and Tanis. The Power9 cluster is a key local investment that enables access to remote facilities at much larger scales by supporting proofs-of-principle and key findings ahead of further scale-up and scale-out on leadership-class machines available in Department of Energy (DOE) facilities (such as ORNL and Lawrence Livermore National Laboratory (LLNL)). This system also supports small-scale parallel modeling and simulation, containerization of codes and data. The performance-portability issues of such scalable codes can be identified, at least in part, only with dedicated local resources of this scale (about 1/1,000th the size of ORNL's Summit). A two-day seminar was held at SimCenter on Machine Learning based on this technology, which brought UTC students and faculty together with IBM experts and visitors from regional universities. Important classes of machine learning and data analytics are also greatly enabled by this system.

As of October 2018, the investment in this cluster has enabled new collaborations with the University of Tennessee at Knoxville (UTK): Dr. Michela Taufer and Dr. Skjellum are teaming on data analytics and Message Passing Interface research with anticipated external, joint funding in FY2019 from DOE; Dr. Jack Dongarra (UTK) and his research team have started utilizing this cluster in support of their exascale computing work to optimize mathematical libraries.

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

This document constitutes the Annual Report for Fiscal Year 2018 of CEACSE activities and efforts. On behalf of UTC, SimCenter, CECS, our community partners and stakeholders, and our CEACSE-funded scientists and students, we express our deep appreciation to THEC for this critically important support of the CEACSE.

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FACULTY & STAFF

The Center of Excellence in Applied Computational Science and Engineering benefits from institutional leaders who are deeply committed to enriching and expanding computational science as a research area and as an enabler of innovative research across academic departments. The THEC Chair of Excellence is Dr. Tony Skjellum, who joined the UTC in August 2017. CEACSE also partners with Dr. Joanne Romagni, UTC's Vice Chancellor for Research, and Dr. Reinhold Mann, SimCenter Director Emeritus. Please see the **Leadership Contact Information and Bios** section for details of leadership personnel.

CEACSE FY2018 Awardees

The following faculty and staff were integral to the strategic direction of CEACSE during the 2017–18 competition cycle. As noted below, these individuals served as a Lead PI and/or Co-Investigator on projects that advanced the CEACSE mission and vision. Biosketches for all faculty may be found in **Appendix A**.

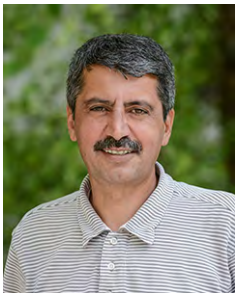
Dr. Neslihan (Nesli) Alp*

Dr. Nesli Alp is a Professor and Department Head of the Engineering Management & Technology Department and Associate Dean of the College of Engineering and Computer Science (CECS). She holds the Chattanooga Manufacturers Association (CMA) Chair position in CECS. Dr. Alp earned a Ph.D. in Engineering Management from the University of Missouri-Rolla (Missouri University of Science & Technology) (1996), a master's degree in Industrial Engineering, and a bachelor's degree in Engineering Management from Istanbul Technical University, Turkey. Her teaching and research areas are project management, quality control, facilities management, optimization, lean systems, manufacturing processes, and distance education. She is a member of the American Society for Engineering Management (ASEM), American Society of Engineering Education (ASEE), Industrial and Systems Engineering (ISE), American Society of Quality (ASQ), Project Management Institute (PMI), and Society of Women Engineers (SWE). She previously served as the faculty advisor for UTC's SWE student chapter. She strongly advocates for women and other minority students in the STEM field. Please see Dr. Alp's biosketch in **Appendix A** for further information.

Co-Investigator:
"Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings"

**Left UTC at the end of FY 2018.*

Dr. Abdollah (Abi) Arabshahi



Dr. Abi Arabshahi is a Research Professor in the Mechanical Engineering Department; he is primarily housed in the SimCenter. He received a B.S. (1982) in Civil Engineering and an M.S. (1985) and a Ph.D. (1989) in Aerospace Engineering from Mississippi State University. His research interests include computational fluid dynamics, unsteady viscous flow applications, structured and unstructured grid technologies, autonomous underwater vehicles, internal and external aerodynamics and hydrodynamics, and computational bio-fluid dynamics. He has multiple publications in internationally reputable journals and conferences, as well as a book chapter, including *Frontiers of Computational Fluid Dynamics*, *AIAA Journal of Spacecraft and Rockets*, *International Journal of Computational Fluid Dynamics*, *Applied Mathematics and Computation*, *International Journal of Systems*, *Journal of Franklin Institute*, *International Journal of Control*, and American Institute of Aeronautics and Astronautics (AIAA) and American Society of Mechanical Engineers (ASME) conferences. He is a member of Tau Beta Pi (Engineering Honor society), Phi Theta Kappa (Honor Society), AIAA, and ASME. Please refer to Dr. Arabshahi's biosketch in **Appendix A** for more information.

Co-Investigator:
"Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs"

"Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications"

Dr. Feng Bao*

Dr. Feng Bao is an Assistant Professor in the Department of Mathematics. He received a B.S. (2006) in Mathematics from Zhejiang University (Chu Kochen honor class), China; an M.S. (2009) in Probability and Statistics from Shandong University, China; and a Ph.D. (2014) in Mathematics from Auburn University. His research interests include analysis and numerical solutions for stochastic differential equations, analysis and numerical solutions for stochastic particle differential equations, uncertainty quantification, data assimilation and inference for stochastic processes, and stochastic optimization. Please refer to Dr. Bao's biosketch in **Appendix A** for more information.

Lead PI:
"Computational Modeling and Uncertainty Quantification for Wave Energy"

**Left UTC at the end of FY 2018.*

Dr. Jennifer Boyd

Dr. Jennifer Boyd is an Associate Professor and Associate Department Head for the Department of Biology, Geology, and Environmental Science. She received a B.S. (1997) in Environmental Science/English (double major) from Allegheny College and an M.A. (2001), M.Phil. (2002), and Ph.D. (2003) in Earth & Environmental Sciences from Columbia University. Her research and academic interests include plant ecophysiology, global change biology, biological conservation, experiential learning, and science writing. Dr. Boyd has authored 15 papers on these areas in refereed journals, the vast majority as first author or as co-author to a student under her advisement. Collectively, she and her students have given more than forty presentations at research conferences and symposiums. Her combined external funding as a PI while at UTC has totaled nearly $1.75 million, including NSF Major Research Instrumentation and Population and Community Ecology Core Program awards. As a co-PI on two CEACSE awards, Dr. Boyd has been exploring the use of computational tools to address ecological questions related to species abundance, with specific focus on species rarity. To date, she has used network analysis to characterize the body of scientific research in this area. Results of this work were presented at the 2018 Ecological Society of America meeting with an associated manuscript in progress. Please refer to Dr. Boyd's biosketch in **Appendix A** for more information.

Co-Investigator:
"The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution"

Dr. David Giles

Dr. David Giles is an Associate Professor for Biology, Geology and Environmental Science. He received a B.A. (2001) in Biology from Maryville College and a Ph.D. (2008) in Biomedical Sciences with a concentration in Microbiology from East Tennessee State University. His research and academic interests involve assessing the impacts of exogenous fatty acids on the membrane composition and virulence of Gram-negative bacteria, with four publications on the topic since 2017. Dr. Giles utilizes microbiology, genetics, and biochemistry to investigate several bacteria of medical importance in response to environmental and host-specific conditions. Please refer to Dr. Giles's biosketch in **Appendix A** for more information.

Co-Investigator:
"A Computational Study of the Impact of Exogenous Fatty Acid Substitutions on the Vibrio cholerae Outer and Inner Membranes"

Dr. Bradley Harris

Dr. Bradley Harris is an Assistant Professor in the Department of Civil and Chemical Engineering at UTC. He received his Ph.D. (2014) in Chemical and Biomolecular Engineering at UTK. He is the Chemical Hygiene Officer for CECS and the faculty advisor for the UTC student chapter of the American Institute of Chemical Engineers (AIChE). His research interests are in bioengineering, specifically the application of chemical engineering principles to biological problems. He is also passionate about undergraduate research and seeks to maintain a laboratory offering opportunities for chemical engineering students interested in bio-related research. His areas of expertise are biochemistry and cellular and molecular biology, with applications in renewable energy and disease pathogenesis. In his current research, Dr. Harris is studying how bacterial pathogens sense and respond to their environment in an effort to improve disease control strategies. This research has been funded by multiple state and internal awards.

Dr. Harris is also interested in engaging local community college students in chemical engineering through the use of cyber-physical systems (CPS). Dr. Harris is actively working to bring online lab stations involving unit operations such as absorption, distillation, heat transfer, fluid flow, and reaction kinetics through the use of Internet of Things. This project has been funded by internal awards and donor contributions, and it is part of a greater effort by UTC and the City of Chattanooga to advance technologies for smart cities by using CPS to manage assets and resources efficiently. Please refer to Dr. Harris' biosketch in **Appendix A** for more information.

Lead PI:
"A Computational Study of the Impact of Exogenous Fatty Acid Substitutions on the Vibrio cholerae Outer and Inner Membranes"

Dr. Ethan Hereth

Dr. Ethan Hereth is an HPC Specialist for the SimCenter at UTC. He received his Ph.D. (2016) in Computational Engineering at UTK. He is in charge of designing, improving, and maintaining all associated hardware, as well as installing, testing, maintaining sundry research software spanning many application areas. His research interests are in Computational Engineering with a focus on Computational Fluid Dynamics and anything related to HPC hardware/software. He is the main point of contact for researchers who want to use the SimCenter's Research Computing facilities. His areas of expertise are CFD, MPI, HPC/Research Computing hardware, and software systems/infrastructure. In his current research, Dr. Hereth is developing automatic mesh generation software for integration of urban GIS data (building footprint data) with CFD software for the study of contaminate propagation and agent based models. Please refer to Dr. Hereth's biosketch in **Appendix A** for more information.

Co-Investigator:
"A Computational Study of the Impact of Exogenous Fatty Acid Substitutions on the Vibrio cholerae Outer and Inner Membranes"

Dr. Zhen Hu

Dr. Zhen Hu is a former Postdoctoral Fellow in the Computer Science and Engineering (CSE) department at UTC. He received Bachelor's Degrees in Electronics and Information Engineering and in Computer Science and Technology from Huazhong University of Science and Technology, Wuhan, China, in 2004. He received a Master's Degree in Communication and Information Systems from Southeast University, Nanjing, China, in 2006 and finally his Doctor of Philosophy in Electrical and Computer Engineering from Tennessee Technological University in 2010. Dr. Hu's research interests include smart grid, smart building, smart health, environment surveillance, intelligent transportation, advanced wireless communications, smart & connected communities, precision medicine, and health-centric urban mobility. Please refer to Dr. Hu's biosketch in **Appendix A** for more information.

Co-Investigator:
"Enabling Wireless 3C Technologies for Smart and Connected Cities"

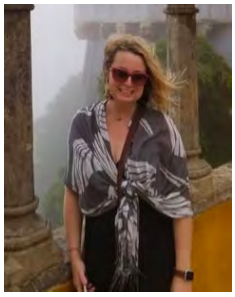
Dr. Farah Kandah

Dr. Farah Kandah is a UC Foundation Associate Professor in the Computer Science and Engineering (CSE) department at UTC. He received his B.S. in Computer Science form the Hashemite University, Jordan in 2002, his M.S. degree in Computer Science from the University of Jordan in 2005, and his Ph.D. in Computer Science from North Dakota State University in 2012.

His research interests and expertise span a wide range of topics in cyber-security and cyber-physical systems networking from stationary wireless networks to ad hoc mobile networks. He is currently leading the Network Communication Laboratory (NCL) at UTC, which leverages expertise on smart communications to support real-time communications in wired and wireless networks, threat-hunting blockchain, and trust management, with research focused on urban science, Internet of Things, public safety, smart networking design, smart autonomous/connected vehicle networks, smart communications, cybersecurity, and Software-Defined Networks. He served as a technical committee member, Co-Chair, and Session Chair for a number of conferences in the field of wireless communications and networking such as CHINACOM, IEEE ICNC, and IEEE CCNC. He also served as a reviewer for several international journals, including *Security and Communication Networks*, *IEEE Sensor Networks*, *International Journal of Information Processing and Management (IJIPM)*, and Journal of Computer Systems, Networks and Communications (JCSNC). Please see Dr. Kandah's biosketch in **Appendix A** for more information.

Co-Investigator:
"Enabling Wireless 3C Technologies for Smart and Connected Cities"

Dr. Hope Klug



Dr. Hope Klug is a UC Foundation Associate Professor and Interim Department Head for Biology, Geology and Environmental Science. She received her B.S. in Zoology and Psychology and her Ph.D. in Zoology in 2007 at the University of Florida. Her research interests include mating systems, social interaction, and parental effort, which are intimately linked to patterns of sexual selection, life-history, and the ways the environment shapes the evolution of different sexes and the selective pressures that affect them. She has multiple publications in a range of internationally reputable journals, including *Frontiers in Ecology and Evolution*, *Nature*, *Ecology Letters*, *Animal Behavior*, and *Evolution*. She also regularly presents her research at international conferences, including the European Society of Evolutionary Biology, the Association for the Student of Animal Behavior, and the International Society for Behavioral Ecology Conferences. Please see Dr. Klug's biosketch in **Appendix A** for more information.

Lead PI:
"The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution"

Dr. Daniel Loveless

Dr. Daniel Loveless is a UC Foundation Assistant Professor of Electrical Engineering at UTC. He received a B.S. degree in electrical engineering from Georgia Institute of Technology, Atlanta, Georgia, in 2004 and M.S. and Ph.D. degrees in electrical engineering from Vanderbilt University, Nashville, Tennessee, in 2007 and 2009, respectively. Prior to joining UTC in 2014, Dr. Loveless was a senior engineer and Research Assistant Professor at the Institute for Space and Defense Electronics (ISDE) at Vanderbilt University. Dr. Loveless has served as PI, Co-PI, or technical lead on programs totaling over $3 million in support. His research interests include radiation effects and reliability in electronic and photonic integrated circuits; high-performance and radiation-hardened digital, mixed-signal, and analog integrated circuit design; embedded systems; field-programmable gate arrays (FPGAs); microprocessors and microcontrollers; systems-on-chip; CubeSat design; sensors; Internet of Things; and smart cities. Dr. Loveless has published over 87 articles in peer-reviewed journals, has been cited over 1400 times, and is a Senior Member of IEEE. His honors include five best conference paper awards, the IEEE Nuclear and Plasma Sciences Society (NPSS) Graduate Scholarship Award for recognition of contributions to the fields of nuclear and plasma sciences, and the Georgia Tech Alumni Association Scholarship. Please see Dr. Loveless's biosketch in **Appendix A** for more information.

Co-Investigator:
"Unlocking the Secrets of RF-DNA Fingerprinting"

Dr. Soubantika Palchoudhury

Dr. Soubantika Palchoudhury is an Assistant Professor in the Civil and Chemical Engineering department at UTC. She received her Ph.D. (2012) in Chemical Engineering at the University of Alabama. Prior to joining UTC, she was a Postdoctoral Researcher at Yale University, the University of South Carolina, and the University of Alabama. Dr. Palchoudhury's areas of interest include nanochemistry, biohybrid nanoarchitectures, semiconductor nanocrystals for photovoltaics, environmental nanoscience, and material characterization, especially transmission and scanning electron microscopy. Dr. Palchoudhury has authored 25 journal articles, four book chapters, and one book in these areas. She serves as an editorial board member, special issue editor, and reviewer for several nanoscience journals. She has received two CEACSE awards for her collaborative computational work with the SimCenter. Dr. Palchoudhury's Integrated Nanobiomaterials research team includes a diverse pool of talented graduate and undergraduate researchers. The group focuses on materials, chemistry, computational, biological, and environmental aspects of nanotechnology. Please refer to Dr. Palchoudhury's biosketch in **Appendix A** for more information.

Lead PI:
"Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs"

Dr. Hong Qin

Dr. Hong Qin is an Associate Professor in the Department of Computer Science and Engineering and the Department of Biology, Geology and Environmental Science. He uses computational and mathematical approaches to investigate biomedical and biological questions. One focus is to develop probabilistic gene network models to infer network changes during cellular aging. He builds gene network models from heterogeneous genomics data sets, including protein interactions, gene expression data sets, RNAseq data sets, protein mass-spec data sets, high-throughput phenotypic screens, and gene annotations. He is also developing machine learning methods to automatically estimate cellular lifespan from time-lapsed images and applying engineering principles to study molecular, biological, and ecological networks. He is developing deep learning methods for better classification and prediction with heterogeneous biomedical and biological large data sets. Dr. Hong Qin is the recipient of an NSF CAREER award (2015–2020) and the lead PI of an NSF Big Data Spoke award (2018–2021). Dr. Qin's areas of expertise are graph reliability modeling, bioinformatics, computational genomics, mathematical modeling, systems biology, cellular aging, and gene network analysis and modeling. Please refer to Dr. Qin's biosketch in **Appendix A** for more information.

Lead PI:
"Connecting the Control Theory of Engineering to a Network Theory of Cellular Aging in Biology"

Co-Investigator:
"The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution"

Dr. Donald Reising

Dr. Donald R. Reising is an Assistant Professor of Electrical Engineering at UTC. He received his B.S. degree in Electrical Engineering from the University of Cincinnati in 2006. He received his M.S.E.E. (2009) and Ph.D. (2012) in Electrical Engineering from the Air Force Institute of Technology. His research interests include wireless device discrimination using RF-DNA fingerprints, digital communications, digital signal processing, and compressive sensing. He is a member of Eta Kappa Nu, Tau Beta Pi, and a senior member of IEEE. Please refer to Dr. Reising's biosketch in **Appendix A** for more information.

Lead PI:
"Unlocking the Secrets of RF-DNA Fingerprinting"

Dr. Mina Sartipi

Dr. Mina Sartipi is the Founding Director of the Center for Urban Informatics and Progress (CUIP) and is also a UC Foundation Professor in the Computer Science and Engineering Department, where she leads the Smart Communications and Analysis Lab (SCAL). She received her B.S. in Electrical Engineering from Sharif University of Technology, Tehran, Iran, in 2001 and her M.S. and Ph.D. degrees in Electrical and Computer Engineering from Georgia Tech in 2003 and 2006, respectively. Dr. Sartipi's research interests are in the area of communications and data science, in particular advanced wireless communications and data analysis for smart healthcare and urban futures. She has served as the technical program chair of conferences in the areas of wireless communications and networking.

In 2008, she was named UC Foundation Assistant Professor. This award was given to her based on her research activities and students evaluating her teaching. She was awarded the UTC Outstanding Faculty Research and Creative Achievement award in 2016. She has also been awarded the best researcher in the CSE department and CECS in 2010, 2013, 2014, and 2015. Dr. Sartipi has been an IEEE senior member since 2016. She has been a member of the Board of Directors for the Enterprise Center, Chattanooga, Tennessee, since 2017. Since 2013, Dr. Sartipi has been a member of the Board of Directors for Variable, Inc., Chattanooga, TN. Please see Dr. Sartipi's biosketch in **Appendix A** for more information.

Lead PI:
"Enabling Wireless 3C Technologies for Smart and Connected Cities"

Dr. Kidambi Sreenivas

Dr. Kidambi Sreenivas is an Associate Professor in Mechanical Engineering. He has been active in the area of unstructured, multi-physics flow solvers since 1996. Prior to this, his focus was in the area of structured flow solver development with applications to acoustics and stability of turbomachinery. Dr. Sreenivas pioneered the capability to enable rotating machinery simulations using unstructured meshes. Additionally, he has developed pre-conditioners that enable simulations of fluids with non-ideal equations of state. Dr. Sreenivas has applied these advanced capabilities to solve real-world problems involving complex geometry and complex physics. The range of applications includes maneuvering submarines and surface ships, simulations of wind farms, multi-stage turbomachinery, improvement in aerodynamic efficiency of Class 8 trucks, particle deposition within the human respiratory system, contaminant dispersal through urban environments, and embedded propulsion systems. Dr. Sreenivas has worked closely with researchers from NASA, the US Navy, the DOE, and various private companies. He has transitioned the latest developments to provide them with advanced flow simulation capabilities. Please see Dr. Sreenivas' biosketch in **Appendix A** for more information.

Lead PI:
"Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications"

Co-Investigator:
"Computational Modeling and Uncertainty Quantification for Wave Energy"

Dr. Craig Tanis

Dr. Craig Tanis is an Assistant Professor in Department of Computer Science and Engineering. He received his BSE in Computer Engineering and M.S. in Computer Science from Tulane University in 1997 and 1998, respectively. He received his Ph.D. in Computational Engineering from UTC in 2013. Dr. Tanis researches the use of programming language techniques in HPC, helping application scientists develop correct codes without compromising computational efficiency. His expertise lies in HPC, programming languages, and interactive multimedia. Please see Dr. Tanis' bio-sketch in **Appendix A** for more information.

Co-Investigator:
"Connecting the Control Theory of Engineering to a Network Theory of Cellular Aging in Biology"

Dr. Endong Wang

Dr. Endong Wang is an Assistant Professor in the Department of Engineering Management & Technology at UTC. He obtained his Ph.D. in Construction Engineering from the University of Nebraska, Lincoln. Before joining UTC, he worked as a Postdoctoral Researcher in Mechanical Engineering at the University of Wisconsin, Milwaukee. His research interests include sustainable construction, building energy performance evaluation, thermal detection, decision making, and environmental assessment. He has teaching experience at both undergraduate and graduate levels in both the US and China. He has been on the review boards of multiple journals and the technical committees of several international conferences. Please refer to Dr. Wang's biosketch in **Appendix A** for more information.

Lead PI:
"Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings"

Dr. Jin Wang

Dr. Jin Wang is Professor and UNUM Chair of Excellence in Applied Mathematics at UTC. He obtained his Ph.D. in Computational and Applied Mathematics from The Ohio State University in 2004. Before joining UTC, he worked at Duke University and Old Dominion University. His research interests include mathematical modeling, numerical analysis, scientific computing, mathematical biology, and fluid dynamics. Please refer to Dr. Wang's biosketch in **Appendix A** for more information.

Co-Investigator:
"Computational Modeling and Uncertainty Quantification for Wave Energy"

FY2018 STUDENTS

Project Title: Computational Modeling and Uncertainty Quantification for Wave Energy
Lead PI: Feng Bao

Students Impacted:

Robert Slaughter, M.S. student: Supervised by Dr. Bao while doing research in stochastic modeling and computation

Chayu Yang, Ph.D. student in Applied/Computational Math: Mentored by Dr. Wang and expected to graduate in 2019

Conrad Ratchford, M.S. completed in spring 2018: Mentored by Dr. Wang and expected to enter UTC's Applied/Computational Math Ph.D. in Fall 2018

Project Title: The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution
Lead PI: Hope Klug

Students Impacted:

Braley Gentry, B.S. student in Biology: Co-led network analysis research related to species rarity. This student is expected to be a co-author on at least one publication and is a co-author on two presentations.

Destinee Jones, B.S. student in Biology, graduated May 2018: Assisted with data extraction and organization related to evolutionary ecology research. This student has been accepted to a graduate program.

Zachary McCoy, M.S. student in Environmental Science, with plans to complete his Ph.D. in Computational Science: Conducted research related to the use of network analysis in evolutionary biology. This student will likely be the first student from our department to pursue a Ph.D. in Computational Science. He is expected to be the lead author on at least one CEACSE-related publication and is a co-author on two presentations related to this project.

Madelyn Momchilov, B.S. student in Biology, graduated May: Assisted with life-history, mating, and parental investment data extraction and organization.

Zachary Sheckley, B.S. student in Biology, graduated May 2018: Assisted with data extraction and organization related to evolutionary ecology research. This student is expected to be a co-author on at least one publication.

Kaitlyn Smith, B.S. student in Biology: Assisted with data extraction and organization related to species rarity research.

Kaitlin Sons, B.S. student in Biology: Assisted with data extraction and organization related to species rarity research.

Thomas Wiegand, B.S. student in Biology: Co-led network analysis research related to species rarity. This student is expected to be a co-author on at least one publication and is a co-author on two presentations.

Project Title: Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs

Lead PI: Soubantika Palchoudhury

Students Impacted:

Uday Gharge, M.S. student in Chemical Engineering, Thesis track, graduated May 2018

Abdulaziz Albattah, M.S. student in Chemical Engineering, Project track, graduated August 2018

Justin Miller, B.S. student in Chemical Engineering, graduated May 2018: Gained experience in wet chemical synthesis, material characterization, conference presentations, and journal publication. This project led to his job at WR Grace Chattanooga.

Ketan Patel, B.S. student in Chemical Engineering, graduating December 2018: Gained expertise in nanomaterial synthesis, agricultural application of nanoparticles, conference presentations, and journal publication.

Olivia George, B.S. student in Chemical Engineering, graduating May 2019: Part of training and research for departmental honors thesis. It has also helped develop scientific communication skills through conference presentations and journal publication.

Erin Conway, B.S. student in Chemical Engineering, graduated December 2017: Gained expertise in multiple hands-on laboratory skills (e.g., nanomaterial synthesis, material characterization techniques), project leadership, teamwork, scientific writing, and conference presentations.

Cody Flowers, B.S. student in Chemical Engineering, graduated May 2018: Gain experience in different nanomaterial synthesis applications, independent research, and method development. Cody is currently working as an engineer at Collider Tech in Chattanooga

Project Title: Connecting the Control Theory in Engineering to a Network Theory of Cellular Aging in Biology
Lead PI: Hong Qin

Students Impacted:

Brittany Campbell/Thomas, B.S. student in Biology: Presented research on UTC Research Day and entered graduate school at UTHSC to pursue a Ph.D. degree.

Project Title: Computational Modeling and Uncertainty Quantification for Wave Energy
Lead PI: Donald Reising

Students Impacted:

Ahmed Ibrahim, M.S. student in Electrical Engineering: Conducted all of the work related to configuration of the HackRF One SDR to transmit and receive using the IEEE 802.11a Wi-Fi. This work has served to introduce him to the RF-DNA fingerprinting process. This work has provided invaluable and necessary experience in scoping and conducting research.

Bharat Patel, M.S. student in Electrical Engineering: Assisted in the work related to the HackRF One SDR and established the initial CFO manipulation protocol using the Max2837 and Si5350 COTS. This work has linked to his M.S. thesis work on the use of RF-DNA fingerprinting for assessment of ionizing radiation degradation (Ionizing Radiation Effects Spectroscopy), which has resulted in one conference presentation and a journal submission. This work has provided invaluable and necessary experience in scoping and conducting research.

Project Title: Enabling Wireless 3C Technologies for Smart and Connected Cities
Lead PI: Mina Sartipi

Students Impacted:

Dr. Khashayar Kotobi, postdoctoral research fellow under Dr. Sartipi's supervision: During his time on this project, Dr. Kotobi learned about new research in wireless communication networks and blockchain technology.

Steven Schmitt, graduate student in Computer Science, graduating December 2018: Focused on Software-Defined Networking (SDN) and worked on building the SDN testbed to be used as a platform to test future research in this field.

Dylan Brownell and **Peyton Ball**, both B.S. students in Computer Science: Learned about programming and networking in smart cities contexts.

Project Title: Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications

Lead PI: Kidambi Sreenivas

Students Impacted:

Jhiin Joo, Ph.D. candidate

David Collao, Research Associate, SimCenter

Hannah Gifford, B.S. student in Mechanical Engineering

Juan Hernandez, B.S. student in Mechanical Engineering

Project Title: Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings
Lead PI: Endong Wang

Students Impacted:

Raghda Mohamed, M.S. student: Learned Building Information Modeling (BIM) for building retrofitting application. She started from knowing little/nothing and now is an expert in BIM use. She used BIM to model one campus building and do retrofitting analysis. With the obtained research results, we have submitted posters to research dialogue and technology symposium at UTC. We are planning to submit a paper to the ASCE conference in Fall 2018.

PROGRAM OVERVIEW & ACCOMPLISHMENTS

The value proposition for multidisciplinary and interdisciplinary research, education, and training in the rapidly advancing field of Computational Science and Engineering[2] (CSE) has grown stronger since the start of CEACSE in 2005. Today, modeling, simulation, and HPC are considered the third pillar of research, development, and scientific inquiry (in addition to theory and experiment) in a broad spectrum of scientific and technical areas. The THEC investment in CEACSE continues to be critically important for UTC to strengthen ongoing interdisciplinary CSE efforts and to continue to improve competitiveness with respect to extramural funding. The primary objectives of CEACSE are as follows:

- Expand CSE capabilities at UTC,
- Support startup of new research and educational work that broadens and expands the CEACSE base of research expertise, and
- Realize appropriate return on investment by attracting new extramural funding.

FY2018 has been another year of growth and enhancement for CEACSE. The leadership team remained comprised of Drs. Joanne Romagni (Vice Chancellor for Research), Tony Skjellum (SimCenter Director), and Reinhold Mann (Asst. Vice Chancellor for Research). Dr. Mann received promotion to his new role on July 1, 2018, at the end of the fiscal year (he was previously a key consultant to Dr. Romagni). Dr. Skjellum has led the CEACSE efforts for approximately fourteen months as of the date of this report, and he plans to grow and support work consonant with the original proposal to THEC for CEACSE. Continued emphasis on modeling and simulation in CSE, HPC, and data science will ground the strategy of advancing and diversifying the participation of UTC faculty and students in CEACSE projects in FY2019 and beyond. Drs. Romagni, Skjellum, and Mann continue ongoing interactions with Dr. Daniel Pack, Dean of Computer Science and Engineering, in the pursuit of excellence of the CEACSE program as well.

The FY2018 portfolio of CEACSE projects accomplished a number of foundational advancements in detailed R&D for computational solvers, smart cities and urban studies, and electric power; simulation and experimentation in the area of drug delivery and bendable nanotubes; and expanded CSE capabilities in important new application areas keyed in other way to the availability of our new computing infrastructure. Importantly, we were able to fund appropriate research projects in all of the identified research foci (highlighted below), although Aerospace/Defense and Smart Cities remain the largest categories by proposals funded. Health and Biological Systems R&D is now growing rapidly and with great promise: its swim lane now has the most self-identified participants. Energy and Environment is also picking up steam. These areas have been well represented in new external research awards received by CEACSE-funded projects.

Even with the investments from FY2017, it was essential to further modernize the locally available HPC infrastructure at UTC. To that end, we made an approximately $800,000

[2] "Future Directions in CSE Education and Research," report from workshop sponsored by SIAM and the European Exascale Software Initiative (EESI-2), held August 4-6, 2014; Breckenridge, CO – Draft, dated March 11, 2015 available at http://www.eu-maths-in.eu/download/General-International-Studies-Prospective/2015-CSE-report-draft.pdf

investment in FY2018, including approximately $500,000 of CEACSE funds (with an additional $100,000 from the UC Foundation). New storage and backup infrastructure for big data and simulations (approximately 1 Petabyte) was commissioned in December 2017, and the 4-node Power9 cluster came online in March 2018. In particular, this cluster and storage, together with baseline funding for code porting, has enabled our professors and students to solve bigger and harder problems locally while preparing them for access to leadership-class machines outside of UTC, such as the forthcoming ORNL Summit system.

Overall, the combined investment in computing infrastructure and core R&D algorithms and code representations is designed to enable our scientists improve their modeling and simulation capabilities. In particular, such updates help our researchers run flow field simulations that will scale out successfully with performance with great performance-portability, thus helping them target leadership-class machines to solve extremely demanding flow problems, such as hypersonic flows (an area for which there is significant new extramural funding as of FY2017, as noted in the previous report, via a collaboration of the University of Tennessee Space Institute (UTSI), the University of Dayton Research Institute (UTDI), UTK, and UTC).

Program Strategy and Organization

The scientific, technical, and programmatic objectives of CEACSE are aligned with the strategic directions of the research and educational programs at UTC. Figure 1 (below) illustrates the central role CEACSE plays in capability and program development potentially impacting all Colleges at UTC. These strategies intersect with problems of global, national, and regional importance in seven primary focus areas[3]:

- Additive & Advanced Manufacturing
- Aerospace & Defense Simulation
- Cybersecurity & Cyber-physical Systems
- Energy & the Environment
- Health & Biological Systems
- High-Performance Computing
- Smart Cities & Urban Dynamics[4]

These application focus areas were selected based on three important criteria:

- The presence of significant scientific and technical challenges for which there was interest, expertise, and the potential to excel at UTC;
- Clear alignment with educational and workforce development missions of UTC; and
- Opportunities to establish extramural R&D funding that can be realized by UTC researchers in strategic partnerships with collaborators at other institutions.

CEACSE proposals that fit one (or more) of these focus areas are reviewed for technical merit and strategic alignment, which includes scrutiny of a specific plan to develop extramural funding. Beginning in FY2018, important advances in proposal content, process, selection, and peer review were applied across the CEACSE program. All CEACSE proposals now undergo a

[3] Since the end of FY2018, these areas have been renamed/reorganized. To maintain continuity moving forward, the current names (as of October 2018) are used throughout this report,

[4] This area has graduated to its own center, CUIP, effective July 1, 2018.

rigorous external review (single-blind in FY2018 and FY2019; double-blind in FY2020). This enhanced review for all applicants encourages growth whether the proposal is funded or not, providing useful feedback for the project and future proposals in addition to honing the connection between seed-funding investments and their potential for meaningful follow-on extramural funding.

While these focus areas span a wide area of science & technology, all excellent ideas that appear outside of these stated areas are considered as long as they have substantial CSE content—particularly those that address computational experimentation and design, data analytics, and/or machine learning, which are, broadly speaking, all classes of modeling and simulation driven by big data and big computation capabilities.

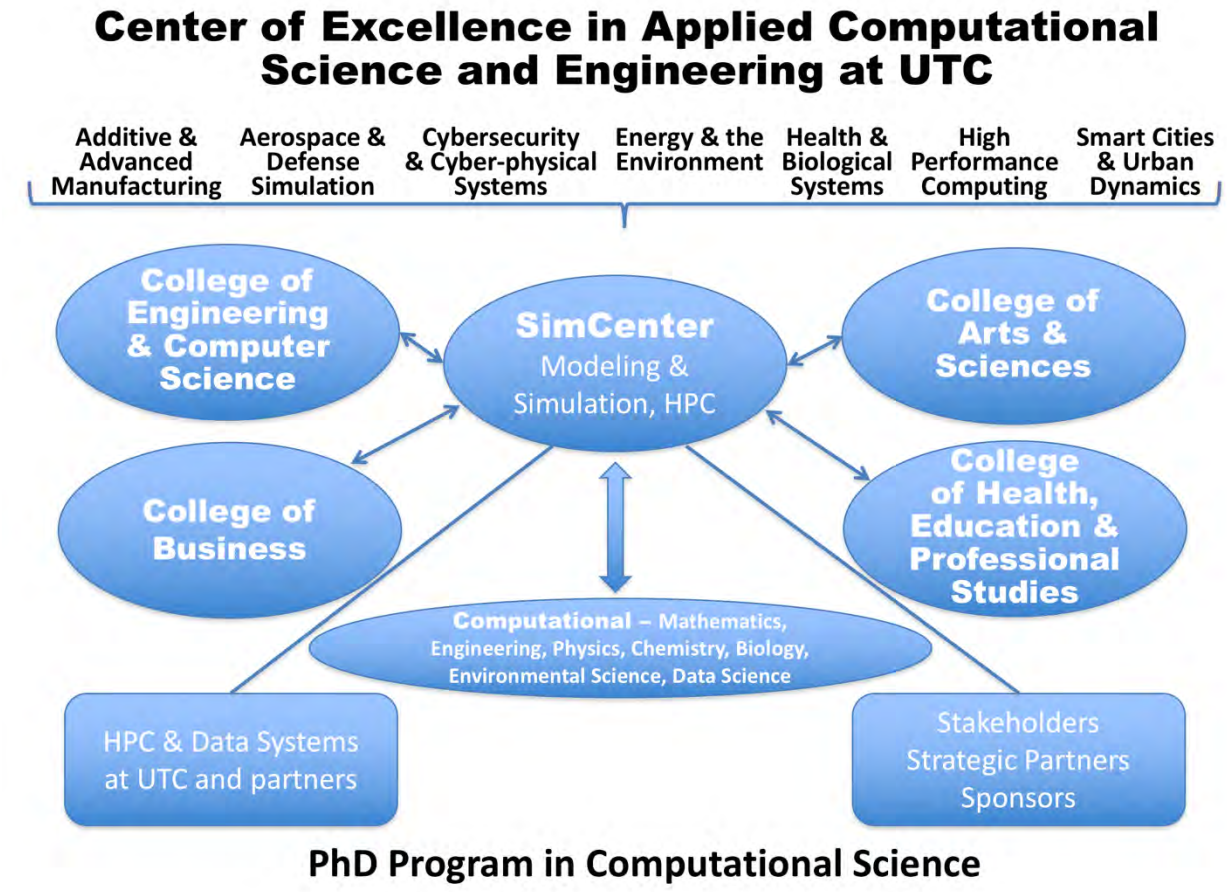


Figure 1: SimCenter serves as UTC's intellectual hub and incubator in modeling, simulation, and HPC in collaboration with departments across campus. Drivers for the activities include the focus areas described in this plan. In addition to CSE, the Ph.D. program now features concentrations in Mathematics and other sciences. Notably, we have achieved further progress toward expanding into Mathematics in the past two years, and there is strong SimCenter participation by math faculty as of Fall 2018 (including one new hire). The THEC Center of Excellence supports cross-disciplinary innovative efforts that are critically important to continued program development, including high-quality faculty recruitment and national competitiveness for follow-on funding.

Overview of FY2018 Projects

In FY2018, CEACSE awarded new seed funding to support the research activities of nineteen faculty members for nine new projects from various disciplines across computational science and engineering. From a total of 29 proposals, these nine were selected for their potential to continue CEACSE efforts to broaden the scope of research through increased participation of additional faculty, graduate students, and undergraduate students.

The funded projects key to the seven CEACSE/SimCenter priority areas: Additive & Advanced Manufacturing, Aerospace & Defense Simulation, Cybersecurity & Cyber-physical Systems, Energy & the Environment, Health & Biological Systems, High-Performance Computing, and Smart Cities & Urban Dynamics. Additionally, certain projects have elements that cross-cut multiple areas, such as Smart Cities & Urban Dynamics plus Energy & the Environment.

Appendix B provides the full Pi-submitted reporting on each of the grants, including detailed final reports articulating the accomplishments, outcomes, and impacts for each award. In addition, Appendix C provides the final reports of two projects hat CEACSE supported prior to FY2018 that were completed in FY2018. The remaining extended projects had minimal additions that were completed within a few months of FY2018 (travel, completing a year of graduate student funding) and thus have no further final report.

Project Title: Computational Modeling and Uncertainty Quantification for Wave Energy
Lead PI: Dr. Feng Bao, Assistant Professor, Department of Math
Co-PI(s): Dr. Jin Wang, Professor, Department of Math

Summary:

Ocean waves, generated by wind blowing over the water surface, have tremendous energy that can be captured and converted into electricity. With the rising demand for energy, growing consumption of oil and gas, and increasing global warming, waves offer an attractive green energy source and have generated considerable interest in research, development, and testing in recent years.

In this project, we focused on the development of computational methods to simulate the complex motion involving ocean waves, wind, and energy buoys. Throughout the past year, the team has conducted extensive work on the computation of wind-ocean wave interaction, fluid-structure interaction, RANS simulation, and stochastic modeling of the fluid motion. In particular, Dr. Bao studied stochastic modeling and numerical solutions for (stochastic) partial differential equations that can be applied to wave energy modeling and wave energy simulations. Dr. Wang's work has been focused on the development of deterministic numerical algorithms for computing multi-phase fluid flows and fluid-structure interactions, essential for the investigation of wave energy dynamics. Dr. Feng Bao and Dr. Jin Wang have submitted three research publications in the award period and generated several new ideas due to the research supported in this project.

Project Title: A computational study of the impact of fatty acid substitutions on *Vibrio cholerae* outer and inner membranes
Lead PI: Dr. Bradley Harris, Assistant Professor, Department of Civil & Chemical Engineering
Co-PI(s): Dr. David Giles, Assistant Professor, Department of Biology, Geology & Environmental Science

Summary:

The bacterium *Vibrio cholerae* (Vc) is responsible for the acute intestinal infection known as cholera. The ability of this pathogen to scavenge lipids from its environment is a crucial factor in how it is able to adapt and spread disease. Our hypothesis is that one way in which Vc utilizes these lipids is for membrane remodeling. To study this hypothesis, we carried out computational simulations of the Vc membranes to analyze the effect of fatty acid substitutions on membrane characteristics. We found that the introduction of exogenous fatty acids causes the outer membrane to become less permeable while also fixing the portions of the membrane susceptible to antibiotics into a more rigid conformation. These findings support our experimental data on Vc membrane permeability and antibiotic resistance in the presence of these fatty acids. Work products from this project include multiple conference presentations, as well as a grant proposal to the National Institutes of Health. A manuscript for submission to a peer-reviewed journal is also currently being drafted. This research has the potential to identify a new class of preventatives and therapeutics for diseases caused by bacterial pathogens. This project supported the mission of the SimCenter by establishing a new multidisciplinary research project in applied computational science in the priority area of health & biological systems.

Project Title: The development and application of computational tools to address fundamental questions in ecology and evolution
Lead PI: Dr. Hope Klug
Co-PI(s): Dr. Jennifer Boyd & Dr. Hong Qin

Summary:

A fundamental goal in biology is to understand both the astounding diversity of life in relation to interactions among organisms and their environment (i.e., ecology) and changes across generations in the genetic and phenotypic makeup of populations (i.e., evolution). Studies of ecology and evolution have significantly advanced our understanding of such diversity; however, most studies thus far have involved the collection and analysis of relatively small datasets. To understand ecological and evolutionary diversity on a large scale, we need to shift our focus to the analysis of large datasets. In recent years, funding agencies and journals have required researchers to deposit data in depositories, which has led to large datasets that can potentially be used to answer fundamental biological questions on a broad scale. However, the unique opportunity to use databases to address broad biological questions is currently hindered by the complication of effectively extracting, sorting, and analyzing their relevant data.

Our CEACSE-related research allowed us to develop and utilize novel computational tools to analyze large datasets extracted from biological databases. Specifically, we first developed and refined computational tools to utilize big datasets. Second, we applied our computational tools to address two fundamental biological questions: 1) What biological traits are linked to species'

rarity, and does rarity influence climate change vulnerability? and 2) How do life-history traits, ecological conditions, and sociality interact to influence mating and parental dynamics?

During the past year, our CEACSE funding allowed us to 1) utilize computing resources to develop novel computational tools and to address pressing questions in ecology and evolution; 2) expand, broaden, and transform the research programs of three faculty members from two departments and colleges; 3) initiate high-impact publications that are currently in preparation for submission; 4) submit several grant proposals; and 5) facilitate the research training of numerous undergraduate and graduate students.

The project advanced the goals of the SimCenter by 1) facilitating computational research, 2) involving faculty from multiple departments and colleges in SimCenter-related research, 3) allowing us to request and secure additional funding for computational research, and 4) training students in computational biology.

Project Title: Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs
Lead PI: Dr. Soubantika Palchoudhury
Co-PI(s): Dr. Abdollah (Abi) Arabshahi

Summary:

Nanodrugs (e.g., Doxil) are seen as a next-generation solution in the field of biomedicine, particularly for their use as chemotherapeutic and drug delivery agents. The key advantage of nanodrugs (at least one dimension < 100 nm) is their ability to selectively reach the diseased site without affecting the healthy tissues. Therefore, a fundamental question in nanomedicine is how to accurately predict the transport and bio-distribution of the new nanodrug within the body. This is nearly impossible to determine from a solely experimental viewpoint. In nanomedicine, a computational approach is used to predict the transport and distribution profile of nanodrugs inside the body, but the method is still in its developmental stages. The goal of this project is to develop a computational model in-house at UTC for predicting the transport of a new Pt-iron oxide nanodrug synthesized at CECS (UTC).

Transport of nanodrugs is a complex process due to the combined involvement of hydrodynamic forces, chemical interaction of the surface, magnetic attraction, adhesion to the cell wall, and Brownian forces. This project developed a robust and preliminary computational fluid dynamics model to predict this transport and to determine the factors dominating the drug's transport. First, physiological geometries for the path of the nanodrug inside the body were generated from literature. Next the mesh or grid was developed through available software. Finally, the flow of the nanodrug was analyzed using *Tenasi*, a flow-solver developed at UTC. Such a model will have immense significance in the biomedical field for designing new and efficient chemotherapeutic nanodrugs. This research directly aligns with the SimCenter's focus area of Health & Biological Systems. The project will put SimCenter at the forefront of emerging innovation in this area. In addition, the project has tremendous potential for publication in high-impact journals due to its novelty. This research has resulted in one article in the reputed journal of RSC Advances. Another article is currently in submission in the AIChE journal. The project also served to provide preliminary data for extramural funding opportunities in NSF and NIH to be pursued collaboratively by the PI and co-PI

Project Title: Connecting the Control Theory in Engineering to a Network Theory of Cellular Aging in Biology
Lead PI: Dr. Hong Qin
Co-PI(s): Dr. Craig Tanis
Other Personnel: Haobo Guo, Postdoc; Emine Guven, Consultant

Summary:

Applying network theories in biomedical research is a promising approach in precision medicine. This project seeks to establish UTC as a national leader in an important new research direction on complex networks. In this project, we prototyped a new algorithm for permutation of networks with power-law features that are found frequently in biology. This new network permutation algorithm enables us to reveal insights on the lifespan extension effect of calorie restriction. A manuscript is under preparation for network configuration analysis. This project has led to cross-disciplinary collaboration of dozens of faculty on UTC campus and multiple external grant applications.

Project Title: Unlocking the Secrets of RF-DNA Fingerprinting
Lead PI: Dr. Donald R. Reising
Co-PI(s): Dr. T. Daniel Loveless

Summary:

The original focus for this effort was to investigate the connection between the waveform distinct and native attributes exploited by the RF fingerprinting process, and the hardware components that form a wireless device's RF front-end. The goals of the project were to 1) identify an individual or set of salient features by which to discriminate an individual device from a much larger population and 2) select and/or develop hardware component models that capture variation(s) of RF front-end components. After award, the focus of the effort was slightly changed based on a Broad Agency Announcement (BAA) from the Defense Advanced Research Projects Agency (DARPA). This BAA was titled "Radio Frequency Machine Learning Systems (RFMLS)" and was focused on the development of a comprehensive approach to developing a machine learning process by which to conduct Specific Emitter Identification (SEI) under various channel conditions and for the case of 10, 100, and 1,000 or more transmitters. In addition, DARPA was interested in the ability to "enhance" transmitter features to ease the process of SEI. Due to the nature of this BAA, Drs. Reising and Loveless teamed up with Pacific Northwest National Laboratory (PNNL) and submitted a proposal under Task 1 – Radio Frequency (RF) Forensics. The UTC team was responsible for Task 1B – RF Waveform Synthesis and PNNL would cover Task 1A – RF Feature Learning. The submitted proposal was not selected for funding; however, based on feedback from the program officer, the focus of the effort was shifted to the generation of preliminary results associated with Task 1B. The purpose of this shift is to facilitate a resubmission of the proposal to another Department of Defense (DoD) agency. Even with this change, the project advanced the SimCenter's work within the area of Smart Cities & Urban Dynamics by looking for a comprehensive and effective means by which to authenticate transmitters and enhance wireless security within IoT. IoT is critical to Smart Cities applications.

Project Title: Enabling Wireless 3C Technologies for Smart and Connected Cities
Lead PI: Dr. Mina Sartipi
Co-PI(s): Dr. Farah Kandah
Other Personnel: Khashayar Kotobi, Postdoctoral fellow

Summary:

We proposed using edge computing and caching to enhance wireless communications in terms of bandwidth and delay by leveraging the concept of mobile 3C systems (communications, computing, and caching (i.e., 3C)). First, we argued that without leveraging concepts of edge computing and caching, the huge burden of data transmission and processing necessary for smart city applications will exhaust current wireless infrastructure. Then we demonstrated the need to merge edge computing with caching to enhance wireless communication for massive data collection in smart cities. To address the security concerns of using IoT in smart cities, we proposed using a blockchain database to secure communication between the smart city and home devices and sensors. This work provided the scalability that is necessary for data transfer between the massive numbers of nodes in IoT that current security protocols do not provide.

The project also focuses on creating a dynamic solution using Software-Defined Networking to meet network needs in supporting high traffic demand. We work on developing a Smart and adaptable network design seeking to utilize network resources more efficiently by identifying traffic patterns and analyzing network metrics to dynamically build virtual slices. With this design, we were able to minimize packet loss, maximize network link utilization, and efficiently reduce the load on the controller. To support the SimCenter efforts in the field of Smart Cities & Urban Dynamics, our team worked on developing an SDN testbed as a proof of concept that can be adopted on a larger scale. The broader impact of this project is its ability to be adopted in different fields in smart cities setups.

Project Title: Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications
Lead PI: Dr. Kidambi Sreenivas
Co-PI(s): Dr. Abdollah (Abi) Arabshahi
Other Personnel: David Collao, Ph.D. (Senior personnel)

Summary:

Noise from various sources is a part of everyday life. The ability to simulate the generation and propagation of noise is a significant challenge. This challenge primarily exists because acoustic waves are a perturbation (very small change) of the ambient pressure, and significant computational resources are required to adequately resolve the flow field. The first step in any of these aeroacoustic simulations is to ensure that one has a good representation of the flow physics and that the relevant noise sources are adequately captured. This adequate capture accomplished through the use of test cases, data that has been obtained through experiments.

Discussions with researchers at the NASA Glenn Research Center and the Naval Surface Warfare Center, Carderock Divison resulted in the identification of two test cases. The turbomachinery test case was simulated using Tenasi, while the flat plate test case was simulated using FUNSAFE. The reason for choosing Tenasi for the turbomachinery simulations is that it is a mature code with significantly more capabilities compared to FUNSAFE.

The turbomachinery test case was the SDT2-R4 fan-stage configuration. This particular stage was designed with three different stator configurations: Baseline, Low-vane, and Low-noise. Earlier simulations of the Baseline configuration were carried out using Tenasi, and good agreement was obtained with experimental data (for overall performance). In the current project, the low-noise configuration was simulated and excellent agreement was obtained with experimental data (overall performance). These simulations involved meshes that contained 104 million nodes and were run on 224 cores of OneSeventeen at the SimCenter. These simulations provided the baseline validation, which was a necessary first step for the acoustic simulations. The results from these simulations were published in a conference paper at the AIAA Aviation 2018 Conference in Atlanta. The flat plate test case is being simulated using FUNSAFE. To obtain the correct pressure perturbations on the surface of the flat plate, LES (Large-Eddy-Simulation) of the flat plate is being carried out. To reduce the computational requirements, these simulations used an approach called rescale-and-reintroduce. This approach had a significant learning curve associated with it; therefore, successful simulations were not obtained in the project time period.

Project Title: Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings
Lead PI: Dr. Endong Wang
Co-PI(s): Dr. Neslihan Alp

Summary:

Effective energy efficiency upgrading through targeted retrofitting on commercial buildings appears to offer a significant opportunity to the overall success of sustainability strategy in the U.S., due to their material share in the totaled building energy consumption of the nation. Per the most recent report of the U.S. Energy Information Administration (EIA), commercial building energy systems consumed 4.29 quintillion joules of primary energy, accounting for more than 38% of those used by stock buildings in the country.

Meanwhile, as an initial departing point, robust fault detection through various diagnosis methods, such as visual inspection, blower door test, infrared thermography, and data-driven benchmarking assumes a nontrivial role in a successful energy retrofitting initiative. Minor errors from the diagnosis process could result in severe mistakes in discovering energy faults and eventually costly failure of an energy retrofitting investment. Nevertheless, the complicated static and dynamic, physical and non-physical interactions among building structure, envelope materials, heating, ventilating, and air conditioning (HVAC), plumbing systems, climate conditions, as well as occupants' behavior, render building energy performance evaluation an uneasy task. The key challenge arises from the dilemma that the pool of energy factors that have been documented to potentially affect energy performance of commercial buildings is extremely large, due to the above complicated concurrent interactions.

Multi-criteria benchmarking is emerging as a more rational option over the traditional single-angle method to assess building performance, which is fundamentally of multifactor nature. Nevertheless, existing multifactor performance diagnosis procedures tend to ignore the common issue of multicollinearity trap, which could result in misleading decisions. Combining with information theory, this project developed models for building energy performance assessment in a multifactor manner to facilitate energy retrofitting programs.

FY2018 Budget

NEW AWARDS FY2018				
Investigators	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Dr. Feng Bao, Dr. Kidambi Sreenivas, Dr. Jin Wang	Computational Modeling and Uncertainty Quantification for Wave Energy	Energy & the Environment	$84,771	$67,977.27
Dr. Bradley Harris, Dr. David Giles, Dr. Ethan Hereth	A Computational Study of the Impact of Exogenous Fatty Acid Substitutions on the *Vibrio cholerae* Outer and Inner Membranes	Health & Biological Systems	$27,481	$27,415.50
Dr. Hope Klug, Dr. Jennifer Boyd, Dr. Hong Qin	The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution	Health & Biological Systems	$97,398	$97,398.00
Dr. Soubantika Palchoudhury, Dr. Abi Arabshahi	Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs	Health & Biological Systems	$99,221	$99,386.03
Dr. Hong Qin, Dr. Craig Tanis	Connecting the Control Theory of Engineering to a Network Theory of Cellular Aging in Biology	Health & Biological Systems	$91,906	$91,905.08
Dr. Donald Reising, Dr. Daniel Loveless	Unlocking the Secrets of RF-DNA Fingerprinting	Smart Cities & Urban Dynamics	$92,062	$87,519.62
Dr. Mina Sartipi, Dr. Farah Kandah, Dr. Zhen Hu	Enabling Wireless 3C Technologies for Smart and Connected Cities	Smart Cities & Urban Dynamics	$92,000	$79,407.02
Dr. Kidambi Sreenivas, Dr. Abdollah (Abi) Arabshahi	Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications	Aerospace & Defense Systems	$68,085	$60,581.97
Dr. Endong Wang, Dr. Neslihan Alp	Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings	Energy & the Environment	$49,902	$46,415.14

AWARDS EXTENDED FROM PREVIOUS AWARD PERIODS INTO FY2018				
Investigators	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Dr. Nur Sisworahardjo, Dr. Abi Arabshahi, Dr. Kidambi Sreenivas	Near Real-Time Detection of Anomalous Power Consumption in Smart Power Distribution Networks	Energy & the Environment	$1,308	$1,308.00
Dr. Craig Tanis, Dr. Kidambi Sreenivas	Optimizing FUNSAFE for Leadership-class Machines	Aerospace & Defense Systems	$8,249	$7,028.19
Dr. Dalei Wu, Dr. Yu Liang, Dr. Li Yang, Dr. Farah Kandah, Dr. Joseph Kizza	Multiscale Serviceability Analysis and Assessment of Urban Infrastructure	Smart Cities & Urban Dynamics	$10,000	$9,999.96
Dr. Daniel Loveless, Dr. Kidambi Sreenivas	Modeling Space and Defense Environmental Effects in Emerging Integrated Circuit Technologies	Aerospace & Defense Systems	$3,581	$3,581

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution:	UTC	Center:	Center of Excellence in Applied Computational Science & Engineering

	FY 2017-18 Actual			FY 2018-19 Proposed			FY 2019-20 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries									
Faculty	$83,672	$155,391	**$239,063**	$324,000	$576,000	**$900,000**	$204,900	$395,100	**$600,000**
Other Professional	$21,618	$40,147	**$61,765**	$36,000	$64,000	**$100,000**	$34,150	$65,850	**$100,000**
Clerical/ Supporting	$760	$1,411	**$2,170**	$18,000	$32,000	**$50,000**	$10,245	$19,755	**$30,000**
Assistantships	$39,554	$73,457	**$113,010**	$54,000	$96,000	**$150,000**	$34,150	$65,850	**$100,000**
Total Salaries	**$145,603**	**$270,405**	**$416,008**	**$432,000**	**$768,000**	**$1,200,000**	**$283,445**	**$546,555**	**$830,000**
Longevity (Exclude from Salaries)	$373	$693	**$1,066**	$2,880	$5,120	**$8,000**	$1,708	$3,292	**$5,000**
Fringe Benefits	$29,691	$55,141	**$84,832**	$108,000	$192,000	**$300,000**	$71,715	$138,285	**$210,000**
Total Personnel	**$175,667**	**$326,239**	**$501,907**	**$542,880**	**$965,120**	**$1,508,000**	**$356,868**	**$688,132**	**$1,045,000**
Non-Personnel									
Travel	$13,685	$25,415	**$39,099**	$13,486	$25,045	**$38,531**	$13,660	$26,340	**$40,000**
Software	$1,283	$2,382	**$3,665**	$6,743	$12,522	**$19,265**	$5,122	$9,878	**$15,000**
Books & Journals	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Other Supplies	$76,139	$141,402	**$217,541**	$9,440	$17,531	**$26,972**	$9,100	$16,250	**$25,350**
Equipment	$143,073	$265,707	**$408,780**	$6,743	$12,522	**$19,265**	$5,250	$9,750	**$15,000**
Maintenance	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Scholarships	$20,104	$37,336	**$57,440**	$26,972	$50,090	**$77,061**	$21,000	$39,000	**$60,000**
Consultants	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Renovation	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Other (Specify):	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Print	$71	$133	**$204**	$111	$205	**$316**	$0	$0	**$0**
Other Personal Services	$3,154	$5,858	**$9,012**	$6,743	$12,522	**$19,265**	$8,750	$16,250	**$25,000**
Membership	$0	$0	**$0**	$135	$250	**$385**	$0	$0	**$0**
Cost Sharing	-$17	-$32	**-$49**	$0	$0	**$0**	$0	$0	**$0**
Group Arranged Events	$118	$218	**$336**	$135	$250	**$385**	$150	$213	**$363**
Special Commercial Services	$2,340	$4,345	**$6,684**	$1,888	$3,506	**$5,394**	$0	$0	**$0**
Total Non-Personnel	**$259,949**	**$482,763**	**$742,712**	**$72,394**	**$134,446**	**$206,841**	**$63,032**	**$117,681**	**$180,713**
GRAND TOTAL	**$435,617**	**$809,002**	**$1,244,619**	**$615,274**	**$1,099,566**	**$1,714,841**	**$419,900**	**$805,813**	**$1,225,713**
Revenue									
New State Appropriation		$766,279	**$766,279**		$781,060	**$781,060**		$820,113	**$820,113**
Carryover State Appropriation		$375,256	**$375,256**		$0	**$0**			**$0**
New Matching Funds	$405,600		**$405,600**	$405,600		**$405,600**	$405,600		**$405,600**
Carryover from Previous Matching Funds	$225,665		**$225,665**	$0		**$0**			**$0**
Total Revenue	**$631,265**	**$1,141,535**	**$1,772,800**	**$405,600**	**$781,060**	**$1,186,660**	**$405,600**	**$820,113**	**$1,225,713**

Schedule 7

FY2018 PUBLICATIONS AND PRESENTATIONS (of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings

J. Wang, "Computing fluid-structure interaction," presented to the Computer Science and Mathematics Division at Oak Ridge National Laboratory, Oak Ridge, TN, September 2017.

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

A. Turgeson, R. Boeger, **D. Giles** and **B. Harris**. "Introducing biochemistry and cellular biology to chemical engineering students by cultivating a bacterial pathogen in a bioreactor," presented at the American Society for Engineering Education Southeastern Section Conference, Daytona, FL, March 2018.

R. Boeger, A. Doyle, **D. Giles** and **B. Harris**. "Studying environmental persistence and virulence factors of Vibrio cholerae in marine and human host environmental conditions," poster presented at the American Institute of Chemical Engineers Southern Regional Conference, Baton Rouge, LA, April 2018.

A. Doyle, R. Boeger, **D. Giles** and **B. Harris**. "Influence of environmental conditions on fatty acid-induced changes in Vibrio cholerae persistence and pathogenicity," poster presented at the Southern Regional Honors Conference, Arlington, VA, April 2018.

B. Harris. "Exploring the impact of the marine-to-host environmental transition on persistence and pathogenicity in Vibrio cholerae using a DOE approach, poster presented at UTC Research Dialogues, Chattanooga, TN, April 2018.

H. Klug, Z. McCoy, **J. Boyd** and **H. Qin**. "Using big data to address fundamental questions in ecology and evolution," poster presented at UTC Research Dialogues, Chattanooga, TN, April 2018.

T. Wiegand, B. Gentry, Z. McCoy, J. Odell, **H. Klug** and **J. Boyd**. "Network Analysis as a method of visualizing connectivity in ecological concepts," poster presented at UTC Research Dialogues, Chattanooga, TN, April 2018.

B. Gentry, T. Wiegand, Z. McCoy, J. Odell, **H. Klug** and **J. Boyd**. "Visualizing connectivity of ecological and evolutionary concepts – an exploration of research on species rarity," poster presented at the Ecological Society of America Conference, New Orleans, LA, August 2018.

U. Gharge, A. Albattah, W. McMahon, M. Rayl, E. Davis, S. Arora, K. Alp, C. Flowers, K. Patel, J. Miller and **S. Palchoudhury**. "Impact of engineered nanoparticles on seedlings," poster presented at NanoBio Summit, Montgomery, AL, November 2017.

U. Gharge, A. Albattah, K. Patel, J. Miller, E. Conway, E. Patrick, O. George and S. **Palchoudhury**. "Impact of engineered nanoparticles on seedlings," poster presented at ACS SERMACS, Charlotte, NC, November 2017.

O. George, W. McMahon, **A. Arabshahi** and **S. Palchoudhury**. "Synthesis and transport of Pt-iron oxide nanodrugs," presented at the National Council of Undergraduate Research Conference, Oklahoma City, OK, April 2018.

S. Palchoudhury, Y. Al Hussain, U. Gharge, A. Albattah and **A. Arabshahi**. "Synthesis and transport of nanoparticle drugs," poster presented at the UTC Technology Symposium, Chattanooga, TN, April 2018.

O. George, K. Patel, W. McMahon, Y. Foster, C. Doumitt, **S. Palchoudhury** and **Arabshahi, A.** "Synthesis and transport of nanodrugs" Research Dialogues, Chattanooga, TN, April 2018.

S. Palchoudhury, **A. Arabshahi**, U. Gharge, A. Boutchuen, Y. Foster, D. Zimmerman and H. Alresheedi, "A new class of integrated chalcogenide nanocrystals and thin films for solar cell applications," submitted to the TMS 2019-148th Annual Meeting & Exhibition, San Antonio, Texas, March 2019.

K. Kotobi and **M. Sartipi**. "Efficient and Secure Communications in Smart Cities using Edge, Caching, and Blockchain," presented at the IEEE Smart Cities Conference, Kansas City, MO, September 2018.

K. Sreenivas. "Computational Simulations of Rotating Machinery," presented at the NASA Glenn Research Center, Cleveland, OH, October 2017.

K. Sreenivas, R. Webster and M. D. Collao. "Computational Simulations of the Low-Noise SDT2-R4 Configuration Using Tenasi," in *Proceedings of the Applied Aerodynamics Conference of the AIAA AVIATION Forum*, 2018.

K. Sreenivas. "Computational Simulations of Low-Noise SDT2-R4 Configuration Using Tenasi," presented at the AIAA Aviation Forum, Atlanta, GA, June 2018.

E. Wang, P. Mao, M. Chen, X. Zhang and L. Li. "Climate effects in data envelopment analysis for residential energy performance benchmarking—An empirical case validation," presented at the ASCE-CRC Conference, New Orleans, LA, April 2018.

M. Cash, **E. Wang** and X. Wang. "Building Information Modeling for Nonresidential Construction—An Industry Perspective," presented at the 2nd International Conference on Applied Mathematics, Modeling and Simulation, Beijing, China, August 2018.

Refereed Publications

Z. Cheng, Y. Liu, M. Zhang and **J. Wang**. "IB-WENO method for incompressible flow with elastic boundaries." *Journal of Computational and Applied Mathematics*, 2018. Acceptance pending on minor revision.

F. Bao, L. Mu and **J. Wang**. "A fully computable posteriori error estimate for the Stokes equations on polytopal meshes". Under review.

S. Palchoudhury, K. Jungjohann, L. Weerasena, **A. Arabshahi**, U. Gharge, A. Albattah, J. Miller, K. Patel and R. Holler. "Enhanced legume root growth with pre-soaking in α-Fe2O3 nanoparticle fertilizer." *RSC Advances*, vol. 8, pp. 24075-24083, 2018.

S. Palchoudhury, **A. Arabshahi**, U. Gharge, A. Albattah, O. George and Y. Foster. "Integrated Experimental and Computational Fluid Dynamics Approach for Nanoparticle Flow Analysis." Under review.

E. Guven and **H. Qin**. "The effect of Gaussian Noise on maximum likelihood inference of survival curves: A comparison of the Weibull and Gompertz models." *Experimental Aging Research*. Accepted.

H. Qin. "Estimating network changes from lifespan measurements using a parsimonious gene network model of cellular aging." *BMC Systems Biology*. Under review.

S. Schmitt and **F. Kandah**. "Denial of Service Attacks Prevention using Traffic Pattern Recognition over Software-Defined Network." *EAI Endorsed Transactions on Ambient Systems*. Under review.

F. Kandah and S. Schmitt. "SAND: Smart and Adaptable Networking Design Using Virtual Slicing over Software-Defined Network." *EAI Endorsed Transactions on Internet of Things*. Under review.

E. Wang. “Decomposing core energy factor structure of US commercial buildings through clustering around latent variables with Random Forest on large-scale mixed data.” *Energy Conversion and Management*, vol. 153, pp. 346–61, 2017.

E. Wang, J. Forst, N. Alp and X. Wang. “Optimizing business operation strategies under uncertainties—A simulation approach.” *Advances in Intelligent Systems Research*, vol. 151, pp. 34–37, 2018.

R. Mohamed, **E. Wang** and X. Wang. “Utilizing BIM for cost estimating in retrofit project.” Drafted.

J. Yuan, L. Li, **E. Wang** and M. Skibniewski. “Examining Sustainability Indicators of Space Management in Elderly Facilities---A Case Study in China.” *Journal of Cleaner Production*. Under revision.

EXTERNAL FUNDING

Dr. Feng Bao, Lead PI

Co-PI(s): Dr. Kidambi Sreenivas and Dr. Jin Wang
Project Title: "Computational Modeling and Uncertainty Quantification for Wave Energy"

Proposal Submissions

1. The team has been collaborating with Dr. Lin Mu (ORNL staff and SimCenter adjunct faculty) in preparation of a joint proposal, partly built on the findings of the current CEACSE project, to the NSF Computational Mathematics program in the near future.
2. Meanwhile, Dr. Wang is currently working with his colleague, Dr. Andrew Ledoan, for a math REU proposal that is to be submitted to NSF in August 2018. Some of the methods and results from this CEACSE project will be incorporated into the proposal.

Contracts/Awards Received

Dr. Bao received the SciDAC (Scientific Discovery through Advanced Computing) project as Co-PI from the DOE during his service at UTC. The SciDAC project is a major research effort intended to encourage collaboration between scientists and computational mathematicians.

Sponsored Program Capacity-Building Activities

The research sponsored in the CEACSE project enhanced SciDAC and other collaborations and improved the capability for faculty to achieve more prestigious research grants.

Dr. Bradley Harris, Lead PI

Co-PI(s): Dr. David Giles and Dr. Ethan Hereth
Project Title: "A Computational Study of the Impact of Fatty Acid Substitutions on the Vibrio cholerae Outer and Inner Membranes"

Proposal Submissions

1. NIH Small Grant Program (R03); PI: Harris; Title: The impact of the marine-to-host transition on fatty acid-induced changes in persistence and pathogenicity in *Vibrio cholerae*; Budget: $100k, Duration: 2 years; submitted February 2018
2. NIH AREA (R15); PI: Wang; Senior Personnel: Giles, Harris; Title: Experimentally guided modeling and simulation for cholera dynamics; Budget: $250k, Duration: 3 years; submitted February 2018
3. FY2019 CEACSE Award; PI: Wang; Co-PIs: Giles, Harris; Title: Waterborne infections and pathogen dynamics: modeling, experimentation, and large-scale computation; Budget: $100k, Duration: 1 year; submitted March 2018

Contracts/Awards Received

1. FY2019 CEACSE Award; PI: Wang; Co-PIs: Giles, Harris; Title: Waterborne infections and pathogen dynamics: modeling, experimentation, and large-scale computation; Award Amount: $100k, Duration: 7/1/18–6/30/19; Sponsor: UTC SimCenter

2. Faculty Pre-Tenure Enhancement Award; PI: Harris; Title: Studying the physiological and behavioral adaptations of pathogenic bacteria in an effort to improve disease control strategies; Award Amount: $15k, Duration: 7/1/17–6/30/18; Sponsor: UTC Office of Research and Sponsored Programs
3. Ruth S. Holmberg Grant for Faculty Excellence; PI: Harris; Title: Studying bacterial physiological and behavioral adaptations in an effort to improve disease treatment and prevention strategies; Award Amount: $5k, Duration: 7/1/17–6/30/18; Sponsor: UTC Provost's Office

Sponsored Program Capacity-Building Activities

Dr. Harris participated in a Grant Writers' Seminar and Workshops (GWSW) grant-writing cohort sponsored by the UTC CECS in Summer 2017, attended the NIH Regional Seminar on Program Funding and Grants Administration in May 2018, and attended two on-campus viewing sessions of NSF CAREER webinars in May 2018.

Dr. Hope Klug, Lead PI

Co-PI(s): Dr. Jennifer Boyd and Dr. Hong Qin
Project Title: "The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution"

Proposal Submissions

1. A Letter of Intent was submitted for the National Science Foundation's (NSF) Rules of Life Program, although a full proposal was not invited.
2. An NSF REU proposal (REU Site: ICompBio - Engaging Undergraduates in Interdisciplinary Computing for Biological Research) was submitted but not funded.
3. An NSF BD Spoke proposal was submitted and has been recommended for funding with Dr. Qin as the lead PI.

Contracts/Awards Received

No awards have been received at this time, but we expect Dr. Qin's BD Spoke proposal to be funded given that it has been recommended for funding.

Sponsored Program Capacity-Building Activities

Co-PI Qin has been in contact with the program officer in relation to the BD Spoke proposal. PI Klug served on an NSF review panel during the grant period.

Dr. Soubantika Palchoudhury, Lead PI

Co-PI(s): Dr. Abdollah (Abi) Arabshahi
Project Title: “Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs”

Proposal Submissions

1. “A New Class of Penternary Chalcogenide Nanocrystals and Thin Films for Solar Energy Conversion Applications” submitted for Oak Ridge Associated Universities Ralph E. Powe Junior Faculty Enhancement Grant, $10,000
2. “Understanding the Effect of Engineered Nanoparticles in Agriculture” submitted for the Center for Integrated Nanotechnologies User Proposal, Sandia National Laboratories

Contracts/Awards Received

Center for Integrated Nanotechnologies User Proposal, Sandia National Lab; Umbrella Non-Proprietary User Agreement

Sponsored Program Capacity-Building Activities

Attendance and meeting with program officers at 2018 NIH Regional Seminar & Pre-Seminar Workshops in Washington, DC

Dr. Hong Qin, Lead PI

Co-PI(s): Dr. Craig Tanis
Project Title: “Connecting the Control Theory of Engineering to a Network Theory of Cellular Aging in Biology”

Proposal Submissions

1. PI Qin submitted an NSF REU proposal on August 23, 2017: "REU Site: ICompBio - Engaging Under-graduates in Interdisciplinary Computing for Biological Research". ~ $359K. This application was declined but was encouraged for resubmission.
2. Qin submitted a proposal to NSF IIS: "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Bio-logical Big Data Research into Student Training and Education", ~$550K, on September 18, 2017. This grant was recommended for funding.
3. An NIH R15, subcontract, was submitted on Oct 25, 2017. Declined.
4. An NSF Rule of Life letter of intent was submitted in January 2018. Declined.
5. The NSF REU was revised and resubmitted on August 22, 2018.

Contracts/Awards Received

No awards have been received at this time, but we expect Dr. Qin’s BD Spoke proposal to be funded given that it has been recommended for funding.

Sponsored Program Capacity-Building Activities

Dr. Qin has been in contact with the program officer in relation to the BD Spoke proposal.

Dr. Donald Reising, Lead PI

Co-PI(s): Dr. Daniel Loveless
Project Title: "Unlocking the Secrets of RF-DNA Fingerprinting"

Proposal Submissions

1. DARPA Microsystems Technology Office BAA: Radio Frequency Machine Learning Systems. August 2017: Release of RFP; October 2017: Full proposal submitted, $2.7M. Not selected for funding.
2. Southeastern Center for Electrical Engineering Education (SCEEE). April 2018: Release of RFP; July 2018: Full proposal submitted, $24,833. Not selected for funding.
3. U.S. Army Communications-Electronics Research Development and Engineering Command (CERDEC), Space and Terrestrial Communications Directorate Solicitation: BAA-18-R-STCD. Open call from 20 June 2018 to 19 June 2023.
    - Two-step solicitation via white paper to determine interest
    - Possible opportunity for re-submission of the DARPA proposal. This proposal would contain preliminary results generated using the resources, lessons learned, processes, and techniques investigated under this CEACSE grant.

Contracts / Awards Received

None

Sponsored Program Capacity Building Activities

Dr. Reising attended the inaugural "Military IoT and Sensors Summit" in Alexandria, Virginia, in May 2018 to get a better sense of the challenges and opportunities for the application of RF-DNA fingerprinting within DoD Internet of Things (IoT) applications. Participation in this summit resulted in connections with Glenn Kesselman from Kesselman & Associates: Cyber Security Products & Services and Dr. Stephen Russell from Army Research Laboratory's (ARL) Battlefield Information Processing Branch. A summary of the developing and ongoing relationship with these two individuals follows.

- Meeting Mr. Kesselman has directly led to Dr. Reising being introduced to Rosetta Cyber Systems, a technology company developing solutions for industrial IoT systems and applications. This introduction has resulted in Mr. Doug Gisby coming to UTC to learn more about the smart building and IoT research being conducted by Drs. Reising, Sartipi, and Loveless. Mr. Gisby expressed Rosetta's interest in conducting a pilot study in the smart building testbed due to be developed and deployed at the SimCenter. Rosetta Cyber Systems is willing to give UTC a copy of their software at no charge, as well as access to necessary data. This opportunity represents a significant collaboration with industry and growth of our smart building research.
- Dr. Russell is the Branch Chief of ARL's Battlefield Information Processing Branch and has a vested interest in the development of "Internet Battlefield of Things" (IBoT). This area includes research and development of IBoT security mechanisms and techniques. He presented the idea and associated challenges at the summit. Currently, Dr. Reising has an ongoing discussion with Dr. Russell over email. We are currently coordinating either a phone or face-to-face meeting. Per Dr. Russell's request, Dr. Reising has shared with him his current MILCOM conference paper that is under review. Dr. Reising will continue to correspond with Dr. Russell in hopes of establishing a source of collaboration and funding of continued work within the area of IoT security using RF-DNA fingerprinting.

Dr. Mina Sartipi, Lead PI

Co-PI(s): Dr. Farah Kandah and Dr. Zhen Hu
Project Title: "Enabling Wireless 3C Technologies for Smart and Connected Cities"

Proposal Submissions

1. NSF S&CC: CI-New: Collaborative Research: A Sandbox for Fostering Smart City Development
2. NSF SaTC: CORE: Small: RUI: vMAP - Mapping Autonomous Vehicle Authentication/Trust Building in Real-time over a Dynamic Adaptive Network
3. NSF CPS: Medium: Collaborative Research: Identity, Trust, and Resilient Architecture for IoT/CPS at Scale

Contracts / Awards Received

None

Sponsored Program Capacity Building Activities

None

Dr. Kidambi Sreenivas, Lead PI

Co-PI(s): Dr. Abdollah (Abi) Arabshahi
Project Title: "Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications"

Proposal Submissions

None (as of now). We're keeping an eye on any upcoming opportunities that are related to the research pursued here and will submit proposals as required.

Contracts / Awards Received

NDA with SmartTruck, Inc., for analysis of flows past Class 8 trucks

Sponsored Program Capacity Building Activities

- Attended the NASA Acoustics Technical Working Group Meeting at NASA Glenn
- Attended the AIAA Aeroacoustics Conference held as part of AIAA Aviation Forum

Dr. Endong Wang, Lead PI

Co-PI(s): Dr. Neslihan Alp
Project Title: "Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings"

Proposal Submissions

1. ORAU: Collaborating with ORNL-DOE (PI), $200
2. UTC: Climate Effects in Residential Energy Performance (PI), $600
3. NSF: Deep Building Energy Benchmarking (PI), $282,560
4. TDOT: Retaining Wall Inspection (PI), $149,857
5. TDOT: Work zone Alert (Co-PI), $174,938
6. TDOT: Open graded Friction Course (Co-PI), $99,996

7. TC: Undergraduate Summer Research (Mentor PI), $5,200
8. NAHB: Homebuilding Education Leadership Program (PI), $100,000

Contracts / Awards Received

1. Oak Ridge Associated Universities: Collaborating with ORNL-DOE (PI), Travel Grant, $200
2. UTC Faculty Development Grant: Climate Effects in Residential Energy Performance (PI), $600
3. Tennessee Department of Transportation: Retaining Wall Inspection (PI), $149,857
4. Tennessee Department of Transportation: Open graded Friction Course (Co-PI), $99,996
5. UTC: Undergraduate Summer Research (Mentor PI), $5,200
6. First Place in Reusable Abstractions of Manufacturing Process (RAMP) National Competition (Team Member, NIST, NSF, ASTM, ASME), Led by Dr. Chris Yuan at Case Western Reserve University

Sponsored Program Capacity Building Activities

- Attended ASCE conference in Louisiana
- Attended Technology Symposium and Research Dialogue

OVERVIEW OF FY2019 PROJECTS

The following awardees and projects, selected for funding in June 2018, are currently supporting CEACSE's strategic goals and future plans in FY2019. All funded projects were subject to single-blind external peer review (reviewers were kept anonymous, but proposers' information remained on their applications), followed by internal panel review in which the external review scores were the driving factor in determining final awards. The SimCenter's grants administrator improved this review process over that of FY2018 by expanding the reviewer search from local (largely UTK) to national (and a few international as well). This change, and further planned improvements, ensure high caliber of funded projects and encourage higher-quality proposals in later competitions. It also has the added benefit of increasing the visibility of UTC and SimCenter outside of Tennessee and planting seeds of possible large-scale collaborations.

Dr. Vahid Rasouli Disfani, Lead PI, in collaboration with Dr. Mina Sartipi and Dr. Mohammad Ahmadi
Awarded $96,114 for "Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design"

Maximizing utilization of electric vehicle supply equipment (EVSE)—or electric vehicle (EV) charging stations—is still a challenge for cities like Chattanooga despite the emergence of EV station locators like PlugShare and ChargeHub. The missing key element in this market is the lack of data from the demand side of EVs, which often leaves EVs desperate for charging not connected while EVSEs are available nearby. This project computationally models and designs an infrastructure that simultaneously gathers demand (EV) data—including desired destinations, connection period, and energy demand—and EVSE availability data to optimally match EVs and EVSEs to maximize social welfare.

Dr. Ignatius Formunung, Lead PI, in collaboration with Dr. Mbakisya Onyango, Dr. Arash Ghasemi, and Dr. Joseph Owino
Awarded $67,568 for "3D Drone Delivery Transportation Problem"

In this work, we consider the realistic model of the three-dimensional motion of a self-controlled drone in a densely populated urban environment. The objective is to deliver packages from multiple points to the multiple destinations using a connected group of drones. The cityscape is first modeled accurately using a tetrahedral grid generated around the GIS data. This grid is then used to determine the connectivity of the destination points. A recent algorithm developed by our team will be utilized to find the minimum routing for each drone. These routes are then corrected by incorporating the wind forces obtained using a computational fluid dynamic (CFD) solver. The idea is to weight the graph such that the drones travel in the wakes of the buildings to have minimum fuel (energy) consumption. We utilize our CFD solver to achieve this goal. Also, we use a 6DOF model for drone and aerodynamic forces obtained by the CFD solver. A simple PID controller is used in each drone to augment the path. The results have vital applications in military data collection by flying spy drones, optimized package delivery using drones, and smart and futuristic cities (where cars can fly!).

Dr. Sumith Gunasekera, Lead PI, in collaboration with Dr. Lakmali Weerasena, Dr. Hong Qin, and Mr. Aruna Saram
Awarded $97,901 for “Estimating the Youden Index under the Multivariate ROC Curve in the Presence of Missing Values of Mass Diseased and Healthy Biomarker Data”

In the context of Binary classification, Receiver Operating Characteristic curves have played an important role in classifying individuals/objects into one of the two predefined classes/populations. These procedures explain how to estimate the Youden index that measures the accuracy of a diagnostic test. However, problem arises when data contains missing values. The proposed research demonstrates how the Youden index for diseased and healthy subjects can be extended to multi-biomarkers in the higher-dimensional space by analytic and extensive computational continuation of the mass missing data of multi-biomarkers from breast cancer and by intensive and extensive computations of the simulated mass data with the aid of the generalized variable method. This computational-extensive mass-data-based procedure is novel and reduces the high number of unnecessary breast biopsies by helping physicians in their decision to perform a breast biopsy on a suspicious lesion seen in a mammogram or to perform a short-term follow-up examination instead. This goal is accomplished by the comparison of classical and generalized variable procedures for the multivariate Youden Index for the multi-biomarkers with missing data, where missing data are cleaned or tackled with imputation using parallel programming procedures in machine learning.

Dr. Farah Kandah, Lead PI, in collaboration with Dr. Mina Sartipi
Awarded $80,000 for “STC3: A Smart Trust-based Connected Autonomous Collaborative Communities”

Connected autonomous vehicles (CAV) are among the key components contributing to Smart City initiatives. Besides communication protocols, securing the network and establishing trust between network entities are among the main challenges that need to be addressed in the field. Securing the network against outsiders’ attacks (trying to bypass the authentication scheme) as well as insiders’ attacks (trying to pollute the network with forged information) are essences to be addressed. Thus, there is both a critical and urgent need to design, prototype, validate, and demonstrate an integrated, real-time system that is better able to ensure the safety of the system by identifying, reporting, and isolating suspicious activities that require immediate attention. In the absence of such information, comprehensive prevention of trust attacks will be impossible, threatening human lives and inhibiting the further development and expansion of the connected and autonomous vehicle industry. The PIs at UTC are uniquely qualified to address the proposed research. Prior work by the team has produced significant early findings that enabled the PIs to design and prototype an effective system. Specific strengths in software-defined networking (SDN) and mmWave enables the team to introduce those concepts as key to improving the proposed trust approach.

Dr. Hope Klug, Lead PI, in collaboration with Dr. Jennifer Boyd, Dr. Azad Hossain, and Dr. Hong Qin
Awarded $99,040 for “Using Computational Tools to Understand the Fundamental Rules of Life”

A fundamental goal in biology is to understand the diversity of life in relation to interactions among organisms and their environment. Most biological studies thus far have involved the analysis of relatively small datasets. To understand diversity on a large scale, we need to shift our focus to the analysis of large datasets. To address the question of why we see striking variation in living organisms, we will use big data and cutting-edge computational tools to 1) enhance our understanding of biological robustness by examining gene/protein interaction networks, 2) explore the factors that make some species rare and other species common, and 3) investigate how abiotic and biotic factors drive the evolution of individual-level traits. In all cases, we will evaluate species network configurations using environmental fluctuations across spatial and temporal scales.

Dr. Lingju Kong, Lead PI, in collaboration with Dr. John R. Graef and Dr. Andrew Ledoan
Awarded $96,380 for “Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations”

The use of social media has been spreading at an accelerated rate in the last decade. Today, there are many social media platforms such as blogs and social network sites. While the dynamics of online social networks have been studied using several models formulated via classical derivatives, these models are local, fail to capture the memory of the system, and have some other deficiencies. The aim of the proposed project is to improve on these studies by utilizing the theory of fractional calculus. Two new dynamic mathematical models based on fractional calculus will be proposed to serve as effective tools for analyzing the mechanisms of online social networks. More precisely, the investigators will first use fractional ordinary differential equations to construct a model to better understand the adoption and abandonment of a social network. Next, they will employ a fractional partial differential equation to model the spatial and temporal characteristics of information diffusion. These models will be compared with real datasets from selected networks. Various model properties such as existence, uniqueness, and stability of solutions will be investigated. Moreover, extensive numerical simulations will be performed to facilitate the analysis and refinement of these models.

Dr. T. Daniel Loveless, Lead PI, in collaboration with Dr. Donald R. Reising
Awarded $99,876 for “Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications”

Process-induced variability and device-level reliability have been identified as bottlenecks to system reliability, introducing a stochastic-nature chip functionality. This disruption necessitates (1) new techniques for measurement of stochastic time-dependent defects; (2) a framework for understanding the dominant device-level reliability failure mechanisms in emerging and disruptive technologies for higher-fidelity predictions of lifetime; and (3) a fundamental understanding of the interplay of variability, operational constraints, and device performance for development of future electronics infrastructure with clear applications in Internet of Things and Space and Defense systems. These goals will be accomplished through the integration of

computational modeling techniques and experimental measurements. We will (1) perform time-dependent defect measurements on advanced FinFET devices; (2) develop stochastic-based models that describe the reliability failure mechanisms and compact models of the time-dependent defects for integration into device and circuit simulators; and (3) provide a novel tool, Ionizing Radiation Effects Spectroscopy (IRES), for measuring the impact of such effects in operational communications systems in situ. This work will offer a fundamentally new approach to evaluating system-level reliability vulnerabilities and has the potential for transforming the way industry assesses electronic device, component, and system reliability.

Dr. Soubantika Palchoudhury, Lead PI, in collaboration with Dr. Abdollah (Abi) Arabshahi
Awarded $100,000 for "Investigating the Flow of Nanodrugs through Bio-Inspired Hydrogel Channels"

Nanodrugs are highly attractive for next-generation medicine because they can be selectively targeted to diseased sites, provide diagnostic capability, and show better solubility compared to conventional therapeutics. However, their transport properties and accumulation within the body are largely unknown, due to experimental challenges in imaging the nanodrugs in complex media. Recently, we developed a combined experimental and computational fluid dynamic approach at UTC to predict the velocity of a new Pt-iron oxide nanodrug through channels of different shapes. In this project, we aim to answer the fundamental question about transport behavior of the nanodrug through custom-designed channels made of materials that closely mimic bronchial airways. The channels will be experimentally developed through two novel approaches: 3D bioprinting and growing different hydrogels within the channel walls. We will develop a computational fluid dynamic model to predict the flow of nanodrugs through these bio-inspired channels for the first time in-house at UTC. The proposed project will have two major outcomes. The computational fluid dynamic model will be a significant breakthrough in drug development and delivery, and using bio-inspired engineering to develop the flow path for nanodrugs will be a key experimental achievement. The project will be used to develop external proposals and publications.

Dr. Hong Qin, Lead PI, in collaboration with Dr. Joey Shaw, Dr. Yu Liang, and Dr. Craig Tanis
Awarded $99,957 for "Analyzing Bioimage Big Data with Deep Learning Neural Networks"

Our goal is to develop state-of-the-art deep convolutional neural networks models (CNNs) to transform two fields of biological research: cellular aging and plant species identification. For cellular aging, we plan to first develop supervised machine learning methods to cluster and label microscopic images for dividing yeast cells. We will then use these labeled images to train CNNs to automatically infer cell division events. For plant species identification, we plan to develop two CNN models and apply them sequentially: the first model will identify plant object regions from herbarium sheets, and the second model will use these objects to classify plant samples into meaningful clusters. Our proposed research will significantly advance the current bioimage big data analytics in these two fields.

Dr. Mina Sartipi, Lead PI, in collaboration with Dr. Nancy Fell
Awarded $99,664 for “Improving Post-Stroke Management Efficiency and Patient Outcomes through Analytics”

For this CEACSE research project, our multidisciplinary team of academic researchers from the Computer Science and Engineering and Physical Therapy Departments will work together to develop a data-driven precision healthcare ecosystem for the management of stroke, the leading cause of long-term disability in the United States. This problem also aligns with the recently launched “big data to knowledge” initiative by NIH. Large-scale multi-modal heterogeneous data and big data analytics are the body and soul of the proposed research, respectively. Data preprocessing, predictive modeling, and prescriptive analytics will be explored and exploited to close the loop of big data analytics for precision healthcare. The computationally intensive concepts, models, algorithms, and functions will be designed and developed to transfer rich data to knowledge—and further to personalized decision support. The proposed inter-professional research will benefit both academic and healthcare communities.

Dr. Kidambi Sreenivas, Lead PI, in collaboration with Dr. Abdollah Arabshahi and Dr. Ethan Hereth
Awarded $77,464 for “Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities”

The overarching goal of the proposed project is to reconstitute the capability (at the SimCenter) to carry out city-scale simulations such that evacuation planning can be carried out. This work will be carried out in collaboration with Dr. Epstein from NYU. The simulations will be carried out using technology developed at the SimCenter, while the agent-based models (ABM) will use agents developed by Dr. Epstein. Upon successful completion, results from this project will be used for an article that is to appear in *Science*. This approach of coupling computational fluid dynamics (CFD) and ABM has applications beyond the proposed project and can be used, for example, to track the spread of pandemics, etc.

Dr. Jin Wang, Lead PI, in collaboration with Dr. David Giles and Dr. Bradley Harris
Awarded $99,992 for “Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation, and Large-Scale Computation”

Waterborne infectious diseases remain a significant public heath burden worldwide. In particular, cholera, a severe intestinal infection caused by virulent strains of the bacterium *Vibrio cholerae*, has expanded in Africa and South Asia and re-emerged in the Americas in recent years as a serious health threat, with an estimated 2–4 million cases per year reported by the World Health Organization. Effective outbreak response and control strategies for waterborne diseases rely on a deep understanding of the pathogen dynamics in reference to the epidemiologic triad of agent, host, and environment. The proposed research aims to establish a new mathematical and computational framework to investigate the pathogen dynamics related to waterborne infections, with a focus on cholera, and to make new discoveries regarding disease transmission and pathogen evolution. The project will combine mathematical models, biological experiments, and advanced numerical methods, with an emphasis on large-scale computation for model implementation and realistic application.

Dr. Weidong Wu, Lead PI, in collaboration with Dr. Jejal Reddy Bathi and Dr. Robert Webster
Awarded $96,217 for “Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems”

Unique properties of engineered nanomaterials (ENMs) have resulted in their increased production. However, it is unclear how these emerging ENMs will move and react once released to the environment. One approach for addressing possible exposure of ENMs in surface waters is by using numerical, mechanistic fate and transport models. There are no reliable fate models currently available that have the ability to simulate ENM behavior in the environment. Our proposed research will explore capabilities of the Environmental Fluid Dynamic Code (EFDC) model, originally developed by the U.S. Environmental Protection Agency (EPA) for simulating hydrodynamics of surface waters, for simulating ENMs. We will examine the model algorithms to address the processes governing ENMs in aqueous media. Since the literature pertaining to type and quantity of ENMs in surface water environment is limited, as the first phase of the proposed research, a systematic evaluation of available literature to identify expected ENMs and their physical, chemical, and biological properties that are important in pollutants fate assessment will be conducted. Second and third phases of the proposed research will include development of a calibrated EFDC model for a river hydraulics and ENM fate simulation under varied scenarios of changed river flows and pollutant loads.

CONCLUSION

CEACSE continues to contribute greatly to the enhancement and expansion of significant and innovative research in computational simulation and applied computational science and engineering. Through THEC's support, CEACSE researchers effectively recognize the special opportunity afforded to UTC to provide leadership in computational applications-driven research and education needed for future competitiveness in the high-technology sector of the global economy. That factor is crucial in their recruitment and retention, as well as professional growth toward tenure and promotion. Significantly, this funding provides a fertile ground to create nationally competitive scholars and research proposals through a peer-reviewed selection process of proposals that are significant enablers of follow-on efforts with extramural funding from NSF, DOD, NASA, and NIH, among others, as well as the potential for industrial sponsorship in certain situations. Those non-federal opportunities appear to be growing with the faculty's growing intellectual property, respective regional/national reputations, and expertise.

Through this seed funding for research activities, undergraduate and graduate students are being engaged in a diverse range of topics at the cutting edge of R&D, and they experience a high level of interaction and involvement with faculty. In coming years, we will also strengthen CEACSE outreach to pre-college students and their teachers.

CEACSE-supported initiatives have already formed the basis of several collaborations and partnerships with other institutions of higher education and with business and industry partners. A number of meaningful Memoranda of Understanding and Non-Disclosure Agreements have been executed between UTC and a variety of partners and potential sponsors to explore how CEACSE can support engineering enhancements, address regional and state priority areas, and bolster robust economic growth. Our strategic partnerships with organizations in Chattanooga and the larger region, such as the Enterprise Center, the CO.LAB, and the Chamber of Commerce have already resulted in increased NSF funds at UTC for CSE-related projects leveraging the Smart-connected GigCity status of Chattanooga.

In conclusion, advancing computational science and engineering to strengthen the education, workforce development, and R&D missions at UTC continues to be a high-value investment for the State of Tennessee and the U.S. The CEACSE multidisciplinary team of faculty and graduate students in collaboration with their strategic partners in Chattanooga, the region, and elsewhere has been focused on the three primary objectives for the Center listed in the introductory segment of this report, namely to

- Expand CSE capabilities at UTC,
- Support startup of new research and educational work that broadens and expands the CEACSE base of research expertise, and
- Realize appropriate return on investment by attracting new extramural funding.

We are convinced that the work accomplished in FY2018 and the strategic vision we have laid out for the future have positioned UTC and CEACSE to continue to positively impact, enhance, and accelerate the growth and advancement of Tennessee's scientific and engineering capabilities and resources.

LEADERSHIP CONTACT INFORMATION AND BIOS

Dr. Joanne G. Romagni

Vice Chancellor for Research & Dean of the Graduate School
Joanne-Romagni@utc.edu

Dr. Joanne Romagni is the Vice Chancellor for Research and Dean of the Graduate School at UTC. Before joining UTC, she was the Associate Vice President for Research at DePaul University in Chicago, where she also served as a research fellow in the biology department. Previously, she held a variety of faculty and leadership positions in research and administration at Bucknell, St. Edwards, and St. Thomas Universities. She received her Ph.D. in plant biology from Arizona State University and conducted research as a postdoctoral plant physiologist and biochemist at the USDA-ARS in Oxford, Mississippi.

In her current role, Dr. Romagni leads efforts at UTC to establish external and interdisciplinary research partnerships to advance the university's strategic plan. Her work develops the structures and support mechanisms to enhance and expand research across graduate and undergraduate disciplines at UTC. Under her leadership, proposal dollars requested have increased by more than $12 million. In FY18, external awards were up by nearly 20% compared to FY17, and Dr. Romagni initiated and administered more than $1,891,986 in internal grant awards.

Dr. Romagni approaches her work with a dedication to synergistic collaboration and strives to provide opportunities to underrepresented individuals. She personally mentored over 75 students in her previous lab, 80% of which were either women and/or Hispanic students. She has developed strong relationships and has extensive experience working with major grant-making agencies, having served on numerous federal review panels. She was awarded funds from the National Science Foundation for her work as a PI developing an international research program for undergraduates. She has been invited by the Association of American Colleges and Universities and the International Conference of Education, Research and Innovation to speak about her expertise and success integrating undergraduate research into curricula.

Dr. Anthony Skjellum

Director of the UTC SimCenter
Chair of Excellence in Applied Computational Science & Engineering
Tony-Skjellum@utc.edu

Dr. Anthony (Tony) Skjellum received his B.S., M.S., and Ph.D. Degrees from Caltech. His Ph.D. work emphasized portable, parallel algorithms and software for simulation, with a specific emphasis on message-passing systems. After graduating in 1990, he worked at LLNL for 2.5 years as a computer scientist, emphasizing performance-portable message passing and portable parallel math libraries. From 1993-2003, he was on faculty at Mississippi State University, where he and his students co-developed MPICH with Argonne National Laboratory, the first implementation of the now-pervasive Message Passing Interface (MPI-1) standard. Skjellum was a leading participant in MPI-1 and MPI-2 standards as well, with specific contributions to the concepts of "groups, contexts, and communicators," which stemmed from

his Ph.D. research. His work on MPI has made broad impact on all HPC worldwide through the MPICH implementation and further R&D on MPI over the past 25 years.

From 2003-2013, he was professor and chair at the University of Alabama at Birmingham (UAB), Department of Computer and Information Sciences, where he continued work on HPC and cyber. During his tenure at UAB, he co-founded a university-wide center, Center for Information Assurance and Joint Forensic Sciences (CIA-JFR), together with Justice Science and Business leaders. This highly funded center was able to attract world-class cybersecurity and forensics researchers. It also spun-off a startup company, Malcovery, which was later acquired by PhishMe and still has a growing presence in Birmingham as of Fall 2018. In July 2014, he was appointed the Lead Cyber Scientist for Auburn University and Cyber Center director. He led the R&D in HPC and cyber at Auburn University in the College of Engineering for just over three years prior to joining the University of Tennessee at Chattanooga in August 2017 as a Professor of Computer Science, Chair of Excellence, and the new SimCenter Director.

Skjellum's current research group is a split between cyber/Internet of Things and HPC and Exascale Storage. FA-MPI is Skjellum's second implementation of a resilient MPI; he and students and his company, MPI Software Technology, previously designed and published MPI/FT, a fault-aware MPI based on MPI/Pro, a commercial MPI licensed from the mid-1990's through mid-2000's. He has current funding from DOE/NNSA and NSF. He is a senior member of ACM and IEEE and Associate Member of the American Academy of Forensic Science (AAFS), Digital & Multimedia Sciences Division. Skjellum remains active in the MPI Forum (in multiple working groups) and is the former chair of the Object Management Group (OMG) High Performance Embedded Working Group as well, in which he remains actively involved as a standards designer and standardizer for high-performance embedded signal and image processing libraries and related application programmer interfaces.

Dr. Reinhold C. Mann

UTC SimCenter Director Emeritus
Reinhold-Mann@utc.edu

Dr. Mann was appointed Deputy Vice Chancellor for Research in July 2018. He has been working with the Vice Chancellor for Research on strengthening collaborations with Chattanooga and the region, most recently with the newly formed Chattanooga Smart Community Collaborative. From 2015 until 2017 he served as the Interim Director of the SimCenter at UTC, a center of excellence in applied computational science and engineering. His work included engaging faculty across UTC in strategy development for the SimCenter as a core capability in modeling, simulation and high-performance computing, ensuring that the strategy remained relevant, and managing program development efforts with potential for sustainable extramural funding for the Center. Mann is also working to promote new collaborative research opportunities between UTC and the UT System (mostly UTK UTSI and UTHSC), and with the Oak Ridge National Laboratory (ORNL).

Mann retired on June 30, 2014 from his position as Associate Laboratory Director for Environmental, Biological and Computational Sciences at the Brookhaven National Laboratory (BNL), where he was responsible for R&D programs in biology, biotechnology, climate science,

and computational science and related efforts. Before joining BNL, Dr. Mann was the Senior Vice President for Research and Development at Battelle Science and Technology Malaysia Sdn. Bhd. in Kuala Lumpur, Malaysia. He moved to this position in November 2008 after leading the Biological and Environmental Sciences Directorate and Program at the Oak Ridge National Laboratory through a five-year period of transformational change with respect to research programs, infrastructure and capability renewal. From 2001 through 2003 he was Deputy Lab Director for Science and Technology, Chief Research Officer, and Associate Lab Director for Fundamental Science at the Pacific Northwest National Laboratory (PNNL).

Dr. Mann's research has been at the intersection of the physical and computational sciences with the life and environmental sciences. He has been leading multi-disciplinary R&D teams since 1986 and developed several R&D efforts in intelligent systems, robotics, human-machine interactions, advanced information processing, computational biology, bioinformatics, systems biology and bioenergy. Dr. Mann served as Chairman of the Board of Directors for the US Department of Energy Bioenergy Science Center in 2007 and 2008, and was a Senior Consultant to the Director of the Oak Ridge National Laboratory from November 2008 through June 2010. Dr. Mann was a member of the Board of Directors for the NASA National Space Biomedical Research Institute, and a member of the Board of Directors for the Laufer Center for Physical and Quantitative Biology at SUNY Stony Brook, from 2011 to 2014. Since June 2015, he has been a member of the Board of Directors for Genera Energy Inc., Vonore TN, a company originally founded to deliver integrated biomass supply chain solutions. Dr. Mann is a member of the Advisory Board at Strata-G LLC, a small business in Knoxville, TN that provides services to help solve complex energy and environmental challenges.

Mann obtained a Diplom-Mathematiker degree (equivalent to an M.S. in Mathematics), and a Dr. rer. nat. degree (equivalent to a Ph.D.) in Physics from the Johannes Gutenberg University in Mainz, Germany. He was awarded a Feodor-Lynen-Fellowship by the Alexander von Humboldt Foundation in Bonn, Germany to do postdoctoral research at the Oak Ridge National Laboratory in 1981 and 1982. He is a Senior Member of the IEEE, and member of the APS and the AAAS.

Appendix A
Faculty Biosketches

Neslihan Alp, Ph.D., P.E.

(a) Professional Preparation

Istanbul Technical University	Istanbul, Turkey	Engineering Management	B.S., 1989
Istanbul Technical University	Istanbul, Turkey	Industrial Engineering	M.S., 1994
University of Missouri-Rolla	Rolla, MO	Engineering Management	Ph.D., 1996

(b) Appointments

2016-Present	**Associate Dean,** Graduate Programs and Research, Department Head of Engineering Management & Technology, & UC Foundation Professor, University of Tennessee at Chattanooga
2014-2015	**Interim Dean**, College of Engineering and Computer Science & UC Foundation Professor, University of Tennessee at Chattanooga
2013-2014	**Associate Dean,** Graduate Programs and Research, Department Head of Engineering Management & Technology, & UC Foundation Professor, University of Tennessee at Chattanooga
2008-2013	**Assistant Dean,** Graduate Programs and Research, Department Head of Engineering Management & Technology, & UC Foundation Professor, University of Tennessee at Chattanooga
2006-2008	**Director of Engineering Management and Graduate Programs** & UC Foundation Associate Professor, University of Tennessee at Chattanooga
2004-2006	**UC Foundation Associate Professor**, College of Engineering and Computer Science, University of Tennessee at Chattanooga
2001 – 2004	**UC Foundation Assistant Professor**, College of Engineering and Computer Science, University of Tennessee at Chattanooga
1999 – 2001	**Assistant Professor**, College of Engineering and Computer Science, University of Tennessee at Chattanooga

(c) Products

(i) Most Closely Related Products

1. **Alp,** N., & Tsai, C. (2014). Using Industry-Sponsored Projects to Improve Outcomes. 34th American Society for Engineering Management International Conference, Virginia Beach, VA, Oct. 15-18.
2. **Alp,** N. & Manning, C. (2014). Creating a Plan for Building Information Modeling. Portland International Center for Management of Engineering and Technology 2014 International Conference Proceedings, Kanazawa, Japan, July 27-31.
3. **Alp,** N. & vonWerssowetz, N. (2013). Integrated Project Development as Applied to Public Projects. Portland International Center for Management of Engineering and Technology 2013 International Conference Proceedings, San Jose, CA, July 28-Aug. 1.
4. **Alp,** N., & Stack, B. (2012). Scope Management and Change Control Process Study for Project-based Companies in the Construction and Engineering Industries. Portland International Center for Management of Engineering and Technology 2012 International Conference Proceedings, Vancouver, Canada, July 29-Aug. 2.
5. **Alp,** N. & Mathai, R. (2010). Smart Grid: A New Approach to Advanced Power Grid and Energy Savings. 31st American Society for Engineering Management Conference Proceedings, Rogers, AR, Oct. 13-16.

(ii) Other Related Products

1. **Alp,** N. & Raymond, D. (2010). Application of Engineering Management Principles to Human Factors Aspect of Nuclear Control Room Design. 31st American Society for Engineering Management Conference Proceedings, Rogers, AR, Oct. 13-16.

2. **Alp, N.** & McGhee, T. (2009). Meeting the Needs of the Construction Industry. 30th American Society for Engineering Management National Conference Proceedings, Springfield, MO, October 14-17.
3. Ware, Jr., J., **Alp, N.,** Cox, R., McDonald, G., & Dreyer, R. (2007). A Continuous Improvement Plan for the Engineering Technology Program in a Community College. 28th American Society for Engineering Management National Conference Proceedings, Chattanooga, TN, Nov. 7-10.
4. **Alp, N.,** Bailey, R., & Pittenger, D. (2007). A Regression Model to Predict the Graduation Rates. American Society for Engineering Education Southeast Section Conference Proceedings, Louisville, KY, April 1-3.
5. **Alp, N.,** Jones, F., Hiestand, J. & Bailey, R. (2006). Use of Taguchi Methods to Optimize the Design of Biomicroreactors. Institute of Industrial Engineers Annual 2006 Conference Proceedings, Orlando, FL, May 20-24.

(d) Synergistic Activities

1. Organized the Project Lead The Way Teaching Training Program held in Memphis and Chattanooga in June and July of 2015.
2. Developed new undergraduate and graduate degree programs, such as Data Science, through the Computer Science & Engineering Department, and the Engineering Management minor through the Engineering Management & Technology Department.
3. Led the selection of the Engineering Management master's program as one of the Best Online Engineering Graduate Programs in the nation, ranking #7 according to US News & World Report.
4. Supported the American Society of Civil Engineers Southeast Student Conference that was hosted by the Civil Engineering Department at UTC in March 2015, impacting more than 1,000 students and faculty from 26 different universities.
5. Established dual degree agreements with local community colleges, such as Chattanooga State, Cleveland State, and Dalton State.

Abdollah (Abi) Arabshahi, Ph.D.

Education:

Ph.D., Aerospace Engineering, Mississippi State University, May 1989
M.S., Aerospace Engineering, Mississippi State University, May 1985
B.S., Civil Engineering, Mississippi State University, May 1982

Professional Experience:

2005 – Present	Research Professor Mechanical Engineering-SimCenter, The University of Tennessee at Chattanooga
2002 – 2005	Associate Research Professor Graduate School of Computational Engineering-SimCenter, The University of Tennessee at Chattanooga
1998 – 2002	Senior Research Associate Applied Research Laboratory, The Pennsylvania State University
1996 – 1998	Research Engineer II, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University
1991 - 1996	Research Engineer I, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University
1989 – 1991	Post-doctoral Fellow, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University

Book:

Whitfield, D. L., Taylor, L. K., Beddhu, M., and Arabshahi, A., "Discretized Newton- Relaxation Solution of theThree-Dimensional Unsteady Incompressible Navier-Stokes Equations," *Frontiers of Computational Fluid Dynamics,* Chapter 28, pp. 575-594, D. A. Caughey and M. M. Hafez, Editors, ISBN 0-471-95334-2, John Wiley & Sons, Ltd., New York, 1994.

Selected Recent Publications (Total 89 Reports and Publications):

1. Hasbestan, J.J., Newman III, J.C., and Arabshahi, A., " Pleasingly Parallel Discontinuous Least Squares Spectral Element Method for Laminar Incompressible Flows with H-Refinement," to be presented at the 55th AIAA Aerospace Sciences Meeting, AIAA Science and Technology Forum and Exposition 2017.
2. Azarnoosh, J., Sreenivas, K., Arabshahi, A., "CFD Investigation of Human Tidal Breathing through Human Airway Geometry," Procedia Computer Science, Vol.80, pp. 965-976, 2016.
3. Hasbestan, J.J., Newman III, J.C., and Arabshahi, A., "PLEASINGLY PARALLEL MATRIX FREE DISCONTINUOUS LEAST-SQUARES SPECTRAL ELEMENT ALGORITHM FOR FLUID FLOW WITH NONCONFORMAL ELEMENT REFINEMENT," FEDSM2016-7510, ASME 2016 Fluids Engineering Division Summer Meeting, Washington, DC, July 10-14, 2016.
4. Azarnoosh, J., Sreenivas, K., Arabshahi, A., "CFD Investigation of Human Tidal Breathing through Human Airway Geometry," International Conference on Computational Science (ICCS), San Diego, California, June 6-8, 2016.
5. Hasbestan, J.J., Newman III, J.C., and Arabshahi, A., "Least Squares Spectral Element Method For Laminar Compressible Flows," AIAA Science and Technology Forum and Exposition (SciTech 2016) San Diego, California, January 4-8, 2016.
6. Gruetzemacher, R., Arabshahi, A."Effects of Inhalation Transience on Particle Transport Through a CT-Based Human Airway Geometry," IMECE2015-52606, International Mechanical Engineering Congress and Exhibition, Houston, TX, November 13-19, 2015.

7. Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Effects of Inhalation Transcience on Flow Structures During Numerical Simulation of Airflow through a CT-Based Airway Geometry," Summer Biomechanics, Bioengineering and Biotransport Conference (SB3C), Snowbird Resort, Utah, June 17-20, 2015.
8. Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Numerical Simulation of Airflow in a CT-based Human Airway Model With Physiologically Appropriate Boundary Conditions," Poster Presentation within the Respiratory Bioengineering Track, Biomedical Engineering Society Annual Meeting, San Antonio, Texas, October 2014
9. Hasbestan, J.J., Newman III, J.C., and Arabshahi, A., "A New Approach to Mesh Adaptation Procedure Using Linear Elasticity for Geometries Undergoing Large Displacements," FEDSM2014-22010, Proceedings of the ASME 2014 4th Joint US-European Fluids Engineering Division Summer Meeting and 11th International Conference on Nanochannels, Microchannels, and Minichannels, Chicago, Illinois, August 2014.
10. Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Simulation of Airflow and Particle Deposition in the Lungs," Poster Presentation, 2014 UT Institute of Biomedical Engineering Symposium, Knoxville, TN , April 2014.

Selected Recent Grants and Contracts (Total 55):

1. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Computational Simulations of the Aerothermal Environment of Hypersonic Fight Vehicles," PI, $97,859.00, July 2016 –June 2017; Funded.
2. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Numerical Simulations of Axial Compressor Flow Fields Employing Higher-Order Accuracy," Co-PI, $96,210.00, July 2016 –June 2017; Funded.
3. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering ,"Towards simulation of vertical axis wind turbines in offshore settings," Co-PI, $100,887.00, July 2016 –June 2017; Funded.
4. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Near Real-Time Detection of Anomalous Power Consumption in Smart Power Distribution Networks," Co-PI, $98,418.00, July 2016 –June 2017; Funded.
5. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "FUNSAFE Framework Development for Enhanced Multidisciplinary and Multiphysics Simulations," Co-PI, $94,684.00, July 2016 –June 2017; Funded.
6. Submitted a research proposal entitled, "Minimizing the impact of gaps on aerodynamic performance of freight trains," to the Tennessee Department of Transportation (TDOT), Co-PI, $250,000.00, March 2016; Not Funded.
7. Submitted a research proposal entitled, "Improving aerodynamic performance of freight trains," to the Tennessee Department of Transportation (TDOT), Co-PI, $250,000.00, March 2016; Not Funded.
8. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Numerical Simulation of Airflow in the Small Human Airways," PI, $100,577.00, July 2015 –June 2016; Funded.
9. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Physics Based Prediction of Stability and Control Characteristics Using Sensitivity-Enhanced Reduced Order Models," PI, $92,533.00, July 2015 –June 2016; Funded.
10. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Predictions of Intracranial Aneurysms Rupture Based on Computational Fluid Dynamics," PI, $99,728.00, February 2015; Not Funded.
11. National Science Foundation,"Towards Understanding Complex Flows Through Bifurcating Networks with Applications to the Human Pulmonary System," PI $296,709.00, Oct. 2015; Not Funded.

Feng Bao

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Office: 417E, Building EMCS

Research Interests

- Analysis and numerical solutions for stochastic differential equations
- Analysis and numerical solutions for stochastic partial differential equations
- Data assimilation and inference for material science
- Uncertainty quantification
- Stochastic optimization

Education

Auburn University, Auburn, Alabama, USA
Ph.D. in Mathematics, August, 2014
- Dissertation Topic: Efficient Numerical Algorithms for Solving Nonlinear Filtering Problems

Shandong University, Jinan, Shandong, China
M.S. in Probability and Statistics, June, 2009
- Thesis Topic: Numerical Solutions of Forward Backward Stochastic Differential Equations and Its Applications in Finance

Zhejiang University, Hangzhou, Zhejiang, China
- B.S. in Applied Mathematics (Chu Kochen honor class), June, 2006

Professional Experience

The University of Tennessee at Chattanooga, TN, USA
Assistant Professor, Department of Mathematics — July, 2016 - present

Oak Ridge National Laboratory, Oak Ridge, TN, USA
Postdoctoral Research Associate, Computer Science and Mathematics Division — July, 2014 - July, 2016

Oak Ridge National Laboratory, Oak Ridge, TN, USA
Intern Researcher (ASTRO program), Computer Science and Mathematics Division — Summer 2013

Auburn University, Auburn, AL, USA
Research Assistant, Department of Mathematics and Statistics — Aug. 2009 - June. 2014

Honors and Awards

DOE Research Grant (PI): $59944, 2016-2017 (awarded); $60000, 2017-2018 (in process)

Astro Internship at Oak Ridge National Laboratory, summer of 2013

Winner of the 37th SIAM SEAS Conference Student Paper Competition, Knoxville, Tennessee, 2013

Don and Sandy Logan Fellowship, Auburn University, 2012 - 2013

Excellence in Research, Department of Mathematics and Statistics, Auburn University, 2012 - 2013

Pending Grant

NSF – Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems (PI)

ORAU Ralph E. Powe Early Career Award (PI)

Projects

Accurate Quantified Mathematical Method for Neutron and Experimental Science (DOE)

Environment for Quantifying Uncertainty: Integrated and Optimized at the extreme scale (DOE)

I-Math: An Interdisciplinary Math Training Platform (NSF)

Publications and Preprints

1. **F. Bao**, Y. Cao and W. Zhao, "*Numerical Solutions for Forward Backward Doubly Stochastic Differential Equations and Zakai Equations*", ***International Journal for Uncertainty Quantification***, 1(4), pp. 351-367, 2011.
2. **F. Bao**, Y. Cao and X. Han, "*An Implicit Algorithm of Solving Nonlinear Filtering Problems*", ***Communications in Computational Physics***, 16(2), pp. 382-402, 2014.
3. **F. Bao**, Y. Cao, C. Webster and G. Zhang, "*A Hybrid Sparse-Grid Approach for Nonlinear Filtering Problems Based on Adaptive-Domain of the Zakai Equation Approximations*", ***SIAM/ASA Journal on Uncertainty Quantification***, 2(1), pp.784-804, 2014.
4. **F. Bao**, Y. Cao and W. Zhao, "*A First Order Semi-discrete Algorithm for Backward Doubly Stochastic Differential Equations*", ***Discrete and Continuous Dynamical Systems - Series B***, 2(5), pp. 1297-1313, 2015.
5. **F. Bao** and Y. Cao, "*Forward Backward Doubly Stochastic Differential Equations and Optimal Filtering of Diffusion Processes*", arxiv:1509.06352
6. B. Hu, Y. Cao, W. Zhao and **F. Bao**, "*Identification of hydraulic conductivity distributions in density dependent flow fields of submarine groundwater discharge modeling using adjoint-state sensitivities*", ***SCIENCE CHINA Earth Sciences***, 59(4): 770-779, 2016.
7. **F. Bao**, Y. Cao, A. Meir and W. Zhao, "*A First Order Fully Discretized Numerical Algorithm for Backward Doubly Stochastic Differential Equations*", ***SIAM/ASA Journal on Uncertainty Quantification***, 4(1), 413-445, 2016.
8. **F. Bao**, R. Archibald, D. Bansal and O. Delaire, "*Hierarchical Optimization for Neutron Scattering Problems*", ***Journal of Computational Physics***, 315: 39-51, 2016.
9. **F. Bao**, Y. Cao, C. Webster and G. Zhang, "*An Efficient Meshfree Implicit Filter for Nonlinear Filtering Problems*", ***International Journal for Uncertainty Quantification***, 6(1), 19-33 2016.
10. **F. Bao**, Y. Tang, M. Summers, G. Zhang, C. Webster, V. Scarola and T.A. Maier , "*Fast and Efficient Stochastic Optimization for Analytic Continuation*", ***Physical Review B***, 94: 125149, 2016.
11. **F. Bao**, R. Archibald, J. Niedziela, D. Bansal and O. Delaire, "*Complex Optimization for Big Computational and Experimental Neutron Datasets*", ***Nanotechnology***, 27(48), 484002 , 2016.
12. **F. Bao**, Y. Cao, X. Han and J. Li, "*Efficient Particle Filtering for Stochastic Korteweg-De Vries Equations* ", ***Stochastics and Dynamics***, 1750008 (2016)
13. K. Kang, V. Maroulas, I. Schizas and **F. Bao**, "*Improved Distributed Particle Filters for Tracking in Wireless Sensor Network*", ***Computational Statistics and Data Analysis***, in revision.
14. **F. Bao** and Y. Cao, "*A Backward Doubly Stochastic Differential Equation Approach for Nonlinear Filtering Problems*", ***Communications in Computational Physics***, submitted
15. **F. Bao** and V. Maroulas, "*Adaptive Meshfree Backward SDE Filter*", ***SIAM Journal on Scientific Computing***, submitted.

Selected Talks and Presentations

SIAM Southeastern Atlantic Section Conference, Tallahassee, FL, March 18-19, 2017

SIAM CSE Conference, Atlanta, GA, February 28 - March 3, 2017

SIAM Southeastern Atlantic Section Conference, Athens, GA, March 5-8, 2016

45th Annual John H. Barrett Memorial Lectures, University of Tennessee, May 14, 2015

Applied and Computational Mathematics Seminar, Clemson Unversity, April 14, 2015

SIAM Southeastern Atlantic Section Conference, Birmingham, AL, March 20-22, 2015

Probability Seminar, University of Tennessee, March 3, 2015

Applied and Computational Mathematics Seminar, University of South Carolina, November 21, 2014

SIAM Conference on Uncertainty Quantification, Savannah, GA, March 31-April 3, 2014

Uncertainty Quantification Group Seminar, Massachusetts Institute of Technology, November 14, 2013

SIAM Annual Meeting, San Diego, USA, July 8-12, 2013

SIAM Southeastern Atlantic Section Conference, Knoxville, TN, March 22-24, 2013

SIAM Southeastern Atlantic Section Conference, Huntsville, AL, March 24-25, 2012

SIAM Annual Meeting, Pittsburgh, PA, July 12-16, 2010

ABBREVIATED CV – Jennifer Nagel Boyd

a. Professional Preparation

Allegheny College	Meadville, PA	Environmental Science & English	B.S., 1997
Columbia University	New York, NY	Earth & Environmental Science	M.A., 2001
Columbia University	New York, NY	Earth & Environmental Science	M.Phil., 2002
Columbia University	New York NY	Earth & Environmental Science	Ph.D., 2003

b. Appointments

2014 – present	Associate Professor, University of Tennessee at Chattanooga (UTC)
2008 – present	Assistant Professor, University of Tennessee at Chattanooga (UTC)
2007 – 2008	Visiting Assistant Professor, Connecticut College
2006 – 2007	Instructor/Laboratory Coordinator, University of Hartford
2003 – 2005	Postdoctoral Fellow, University of Tennessee
1998 – 2003	Graduate Research Fellow, Columbia University

c. Products

(i) 5 most closely related to the proposed project

1. Wilder L[*], **Boyd JN** (2016) Ecophysiological responses of *Tsuga canadensis* (Eastern Hemlock) to projected atmospheric CO_2 and warming. *Southeastern Naturalist* 15: 697-713.
2. **Boyd JN**, Raymond GA[*], Call GP, Pistrang MJ (2016) Ecophysiological performance of the rare terrestrial orchid *Platanthera integrilabia* across contrasting habitats. *Plant Ecology* 217: 1259-1272.
3. **Boyd JN**, Xu CY, Griffin KL (2009) Cost-effectiveness of leaf energy and resource investment of invasive *Berberis thunbergii* (Japanese barberry) and co-occurring native shrubs. *Canadian Journal of Forest Research* 39: 2109-2118.
4. **Nagel JM**[†], Wang XZ, Lewis JD, Fung HA[*], Tissue DT, Griffin KL (2005) Atmospheric CO_2 enrichment alters energy-use efficiency and patterns of energy investment and allocation in *Xanthium strumarium*. *New Phytologist* 166: 513-523.
5. **Nagel JM**[†], Huxman TE, Griffin KL, Smith SD (2004) CO_2 enrichment reduces the energetic cost of biomass construction in an invasive desert grass. *Ecology* 85: 100-106.

(ii) 5 other significant

1. Benson AR[*], **Boyd JN** (2014) Individual- and population-level effects of *Odocoileus virginianus* herbivory on the rare forest herb *Scutellaria montana*. *Global Ecology and Conservation* 1: 80-92.
2. Sikkema JJ[*], **Boyd JN** (2015) Impacts of invasive nonnative plant species on the rare forest herb *Scutellaria montana*. *Acta Oecologica* 69: 182-191.
3. Kile HM[*], Shaw J, **Boyd JN** (2013) Response of federally threatened *Scutellaria montana* (large-flowered skullcap) to pre-transplantation burning and canopy thinning. *Southeastern Naturalist* 12: 99-120.
4. **Nagel JM**[†], Griffin KL, Schuster WSF, Tissue DT, Turnbull MH, Brown KJ, Whitehead D (2002) Energy investment in leaves of red maple and co-occurring oaks within a forested watershed. *Tree Physiology* 22: 859-867.
5. **Nagel JM**[†], Griffin KL (2004) Can gas-exchange characteristics help explain the invasive success of *Lythrum salicaria*? *Biological Invasions* 6: 101-111.

[†] *denotes maiden name;* [*] *denotes student author*

d. Synergetic Activities

1. Integration of student research training into all aspects of my research, including supervision of ~50 undergraduate research assistants and service as the thesis advisor for nine graduate students at UTC (including five who have graduated to date and one who will graduate in spring 2017). Collectively, this research has produced six research articles co-authored by students published in peer-reviewed scientific journals, an additional manuscript with student co-authorship in review for publication, an invited review with student co-authorship in preparation, ten technical reports co-authored by students, and >20 student presentations in scientific venues.
2. Significant institutional service as the Graduate Program Coordinator of the M.S. in Environmental Science program at the University of Tennessee at Chattanooga from 2015-present.
3. Editorial service as the physiology subject editor for *Castanea* from 2012-present and as a reviewer/referee for *Acta Oecologia*, *American Journal of Botany*, *Castanea*, *Ecosphere*, *New Phytologist*, *Plant Ecology*, *PLoS One*, and *Southeastern Naturalist* during the past five years.
4. Regional professional service as an elected member-at-large of the Southern Appalachian Botanical Society since 2015, Botany Section chair of the Tennessee Academy of Science from 2013-2014, Botany Section secretary of the Tennessee Academy of Science from 2012-2013, Chair of the Student Poster Award Committee for the Association of Southeastern Biologists from 2013-2014, and member of the Student Poster Award Committee for the Association of Southeastern Biologists from 2011-2013.
5. Local public outreach including giving the inaugural talk for the *Let's Chatt about Science* Science Café in November 2016, offering a class at the Chattanooga Nature Center called 'Plant Communities' as a core course offering for its Certificate of Native Plants program during July 2014, assisting the Town of Signal Mountain in preparing its successful 2010 application to the Arbor Day Foundation to become a *Tree City USA* and a subsequent renewal application in 2015, and giving interviews in to WUTC (local NPR station) and WDEF (local television station) about local ecological issues in 2013 and 2016.

Curriculum Vitae – David K. Giles

Education

Ph.D.	2008	East Tennessee State University	Biomedical Sciences
B.A.	2001	Maryville College	Biology

Professional Positions

Assistant Professor	University of Tennessee at Chattanooga	2012–present
Lecturer	The University of Texas at Austin	Fall, 2010

Research Activity (past 5 years)

Publications

Madsen, J. A., H. Xu,, M. R. Robinson, A. P. Horton, J. P. Shaw, **D. K. Giles**, T. S. Kaoud, K. N. Dalby, M. S. Trent and J. S. Broadbelt. 2013. High-throughput database search and large-scale negative polarity LC-MS/MS with Ultraviolet photodissociation for complex proteomic samples. *Mol. Cell Proteomics. 12: 2604-2614.*

Pride, A. C., C. Herrera, Z. Guan, **D. K. Giles** and M. S. Trent. 2013. The outer surface lipoprotein VolA mediates utilization of exogenous lipids by *Vibrio cholerae*. *MBio 14: e00305-00313. Co-corresponding author*

Needham, B. D., S. Carroll, **D. K. Giles**, G. Georgiou, M. Whiteley and M. S. Trent. 2013. Modulating the innate immune response by combinatorial engineering of endotoxin. *Proc. Natl. Acad. Sci. USA.* 110: 1464-1469.

Maue, A. M., K. Mohawk., F. Poly, **D. K. Giles**, C. P. Ewing, M. A. Monteiro, M. S. Trent, and P. Guerry. 2013. The polysaccharide capsule of *Campylobacter jejuni* 81-176 modulates the host immune response. *Infect. Immun. 81: 430-440.*

Cullen, T. W., D. R. Hendrixson, **D. K. Giles**, R. I. Hobb, J. O'Brian, S. A. Thompson, J. S. Brodbelt and M. S. Trent. 2013. EptC of *Campylobacter jejuni* mediates phenotypes involved in host interactions and virulence. *Infect. Immun. 81: 665-672.*

Hankins, J. V., J. A. Madsen, **D. K. Giles**, J. S. Brodbelt and M. S. Trent. 2012. Amino acid addition to *Vibrio cholerae* LPS establishes a link between surface remodeling in Gram negative and Gram positive bacteria. *Proc. Natl. Acad. Sci. USA.* 109: 8722-8727.

Manuscripts in Review or Preparation

Moravec, A. R., Siv, A. W., Lindsay, E. N., Shults, D. J., Symes, S. J., and **D. K. Giles**. Exogenous polyunsaturated fatty acids (PUFAs) impact membrane remodeling and affect virulence phenotypes among pathogenic *Vibrio* species. To be submitted Spring 2017.

Baker, L. Y., Siv, A. W., Bible, W. C., Glennon, M. S., Shults, D. J., Symes, S. J., and **D. K. Giles**. Exogenous polyunsaturated fatty acids (PUFAs) impact phospholipid remodeling and virulence phenotypes in *Pseudomonas aeruginosa*. To be submitted Spring 2017.

Eder, A. E., Munir, S. A., Shults, D. J., Symes, S. J., and **D. K. Giles**. Exposure to exogenous fatty acids impacts phospholipid composition, membrane permeability and virulence phenotypes in *Acinetobacter baumannii*. To be submitted Spring 2017.

Selected Undergraduate Research Presentations (past 3 years)

*Anderson, D., *Avello, Z., Symes, S. J. and **D. K. Giles**. 2016. UPLC-MS Characterization of Membrane Phospholipids from *Vibrio* Species Following Exposure to Exogenous Fatty Acids. Southeastern Regional Meeting of the American Chemical Society. Columbia, SC.

*Baker, L. Y. and **D. K. Giles**. 2016. Polyunsaturated Fatty Acids (PUFAs) impact antimicrobial peptide resistance in *Pseudomonas aeruginosa* and *Klebsiella pneumoniae* and cause reduced motility in *P.aeruginosa*. UTC Research Dialogues. Oral Presentation. The University of Tennessee at Chattanooga, TN.

*Schoonover, M. A., *Asemota, S. T., *Avello, Z., *Anderson, D., Symes, S. J. and **D. K. Giles**. 2016. A Survey of Bacterial Biodiversity and Lipid Content within Raccoon Mountain Caverns. Association of Southeastern Biologists Meeting. Oral Presentation. Concord, NC.

*Clavin, M., *Ferrando, B., *Irvin, B., Harris, B. and **D. K. Giles**. 2016. Utilization of Exogenous Lipids: The effects of various fatty acids on *Vibrio cholerae*. UTC Research Dialogues. The University of Tennessee at Chattanooga, TN.

*Munir, S. A., *D. J. Shultz, S. J. Symes, and D. K. Giles. Scavenging Fatty Acids Confers Phenotypic Advantages to *Acinetobacter baumannii*. Oral presentation. National Conference on Undergraduate Research. Eastern Washington University, April 16-18, 2015.

*Eder, A. E., *D. J. Shultz, S. J. Symes, and D. K. Giles. The Effects of Lotion Fatty Acids on *Acinetobacter baumannii*. Oral presentation. National Conference on Undergraduate Research. Eastern Washington University, April 16-18, 2015.

*Siv, A. W., *L. V. Norbash, *D. J. Shults, S. J. Symes and D. K. Giles. Exogenous Fatty Acids Affect Phospholipid Structure, Membrane Remodeling, Biofilm Formation and Susceptibility to Environmental Stress in *Vibrio vulnificus*. Association of Southeastern Biologists Annual Meeting, Chattanooga, TN, April 1-4, 2015.

Grants (past 5 years)

Funded

Harris, B. (PI), **Giles, D**. Physiological and behavioral adaptations of *Vibrio cholerae* to fatty acids in a continuous culture (bioreactor) model. CRISP grant—The University of Tennessee at Chattanooga. **$7,795**

Spratt, H. (PI), Levine, D., **Giles, D**. Environmental Factors Related to Bacterial Nosocomial Infection in Hospital Intensive Care Units in Childrens Hospitals: Assessment and Recommendations for Practice. CRISP grant—The University of Tennessee at Chattanooga. July 2016—June 2017. **$7,958**

Wang, J. (PI), Gao, Liang, Y., **Giles, D.**, Taylor, L., Matthews, M., Liu, Z., Carter, P. NSF Math Infrastructure Program. **$500,000**

Giles, D. (PI), Symes, S. Quantitative and Structural Characterization of Bacterial Phospholipids Following Fatty Acid Exposure. **$8,000**

Giles, D. Environmental DNA and Lipidomic Analyses of Raccoon Mountain Caverns. The University of Tennessee at Chattanooga Research and Creative Activity Grant. July 2015 – June 2016. **$5,057**

Giles, D. Determining the lipid handling capabilities of *Vibrio vulnificus*. The University of Tennessee at Chattanooga Faculty Research Grant. February 2014 – January 2015. **$2,799**

Giles, D. A Proteomics approach to identifying bacterial response pathways to exogenous fatty acids. The University of Tennessee at Chattanooga Summer Fellowship. May – August 2015. **$2,500**

Pending

Giles, D. (PI), Christmann, B. The Impact of Exogenous Polyunsaturated Fatty Acids on Phospholipid Remodeling and Virulence in *Pseudomonas aeruginosa*. **$50,000**

Wang, J. (PI), Heath, G., **Giles, D.**, Harris, B. Mathematical and Computational Modeling of Waterborne Diseases. NIH MIDAS RO1. **$1,165,172**

Wang, J. (PI), **Giles, D.**, Harris, B. Investigating the Pathogen Evolution in Waterborne Enteric Infections. NSF EEID. **$1,022,161**

Bradley Harris

1. **Education**
   - Ph.D., Chemical and Biomolecular Engineering, University of Tennessee at Knoxville, 2014
   - B.S., Chemical Engineering, University of Tennessee at Knoxville, 2008

2. **Academic experience**
   - University of Tennessee at Chattanooga, Assistant Professor, 2015 - Present
   - University of Tennessee at Knoxville, Research Assistant, 2010 - 2014

3. **Non-academic experience**
   - Eastman Chemical Company, Chemical Engineer, oversaw pilot-scale experiments through an outside consultant for research and development of the acetylated wood process, 2008 - 2009
   - Kimberly-Clark Corporation - Berkeley Mill, Co-Op, responsible for several process improvement projects including assessing pellet handling system capacity and conducting mill wide trial of extrusion spinning spray, 2007

4. **Certifications or professional registrations**
   - Registered Engineer-in-Training (EIT)

5. **Current membership in professional organizations**
   - American Institute of Chemical Engineers (AIChE)
   - American Chemical Society (ACS)
   - Tau Beta Pi Engineering Honors Society

6. **Grants, honors and awards**
   - PI, Collaborative Research Initiative for Sponsored Programs (CRISP) Award, University of Tennessee at Chattanooga, 2016-2017 (**$8,000**)
   - Faculty Advisor, Provost Student Research Award, 2016-2017 (**$1,000**)
   - PI, Laboratory Equipment Grant for Chemical Engineering, Tennessee Board of Architectural and Engineering Examiners (TBAEE), 2016 (**$27,000**)
   - Department of Civil and Chemical Engineering Teaching Award, 2015 - 2016

7. **Service activities**
   - Chemical Hygiene Officer, UTC College of Engineering and Computer Science, 2016 – Present: oversee procurement, storage, and disposal of hazardous chemicals; oversee laboratory hazard assessment reviews and safety inspections; ensure proper safety training of faculty, staff, and students
   - Faculty Advisor, UTC AIChE Student Chapter, 2015 – Present: supervise Chem-E-Car student competition team; recruit faculty and industry speakers for monthly meetings; organize plant tours and fundraising activities

8. Publications and presentations

- Clavin, M., Ferrando, B., Irvin, B., Hills, P., Harris, B., and Giles, D. "Bacterial Utilization of Exogenous Lipids: The Effects of Various Fatty Acids on *Vibrio cholerae*." UTC Research Dialogues, Chattanooga, TN, April 13th-14th, 2016.
- Harris, B., Cheng, X., and Frymier, P.D. "The Structure and Function of Photosystem I-[FeFe] Hydrogenase Protein Fusions: An All-Atom Molecular Dynamics Study." *Journal of Physical Chemistry B*, 2016. 120 (4): p. 599-609.
- Harris, B., Cheng, X., and Frymier, P.D. "All-Atom Molecular Dynamics Simulation of a Photosystem I/Detergent Complex." *Journal of Physical Chemistry B*, 2014. 118 (40): p. 11633-11645.
- Le, R., Harris B., Iwuchukwu I.J., Bruce, B., Cheng X., Qian, S., Heller, W.T., O'Neill, H., and Frymier, P.D. "Analysis of the Solution Structure of *Thermosynechococcus elongatus* Photosystem I in n-dodecyl-β-D-maltoside Detergent using Small-Angle Neutron Scattering and Molecular Dynamics Simulation." *Archives of Biochemistry and Biophysics*, 2014. 550-551: p. 50-57.
- Harris, B., Le, R., and Frymier, P.D. "Studying the Effects of Protein-Detergent Interactions on the Solution Structure of Photosystem I from *Thermosynechococcus elongatus*." American Conference on Neutron Scattering, Knoxville, TN, June 4th, 2014.
- Harris, B., Le, R., and Frymier, P.D. "Characterizing the Structure-Function Relationship that Governs Electron Transport in Redox Proteins." ACS Annual Meeting, BIOT Division, Dallas, TX, March 19th, 2014.
- Harris, B., Le, R., and Frymier, P.D. "Photosystem I-Hydrogenase Protein Fusions via Sortase-Mediated Ligation: A Novel Approach to Improving Electron Transport for Photoinduced Hydrogen Production." Best Poster Winner, TN-SCORE Annual Conference, Nashville, TN, June 10th, 2013.
- Harris, B., Frymier, P.D. "Harnessing Solar Energy through Enzyme-Mediated Protein Fusions." ACS Annual Meeting, BIOT Division, New Orleans, LA, April 9th, 2013.
- Harris, B., Frymier, P.D. "Harnessing Solar Energy through Enzyme-Mediated Protein Fusions." Best Poster Winner, TN-SCORE Annual Conference, Nashville, TN, June 15th, 2012.
- Harris, B., Frymier, P.D. "Engineering Protein Fusions for the Photobiological Production of Hydrogen from Light." Eastern Regional Photosynthesis Conference, Woods Hole, MA, April 21st, 2012.

Ethan Alan Hereth

715 Chevoit Dr. Chattanooga, TN 37411
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EDUCATION

Ph.D., Computational Engineering
University of Tennessee at Chattanooga, Chattanooga, TN
Dissertation: *An Automatic Parallel Octree Grid Generation Software with an Extensible Solver Framework and a Focus on Urban Simulation*
Coursework: advanced fluid mechanics, thermodynamics, computational fluid dynamics, adaptive mesh generation/refinement, parallel numerical algorithms, design optimization.

Masters of Science, Applied Mathematics
University of Central Arkansas, Conway, AR, August 2009
Thesis: *Numerical Simulation of Subaqueous Debris Flow in One Dimension*
Coursework: mathematical modeling, advanced ordinary differential equations, numerical analysis, control theory, applied statistics, symmetry analysis of differential equations, advanced partial differential equations.

Bachelor of Science, Applied Mathematics (*Summa Cum Laude*)
University of Central Arkansas, Conway, AR, May 2007
Concentration: Applied Mathematics
Minor: Spanish

EXPERIENCE

High Performance Computing Specialist **December 2016 – Present**
SimCenter at the University of Tennessee at Chattanooga

- Hardware Responsibilities
  - Maintain 350+ diskless HPC servers (approximately 2000 cores)
  - Maintain 500+ port Force10 E1200 switch
  - Maintain one Petabyte storage array
  - Maintain multiple mission critical infrastructural/service servers
    - maintain services like NIS, DHCP, NTP, VPN, CUPS, SNMP
  - Tape backup hardware
  - Maintain dozens of Linux and Windows desktops
  - Familiar with Infiniband technology
- Software Responsibilities
  - Maintain and modify HPC environment monitoring software
  - Manage multiple filesystems running over NFS
  - License managers
  - Planned and implemented a Linux OS/software upgrade for SimCenter desktops
  - Manage (add/delete/modify) user accounts
  - Adept with package managers and software compilation/installation
  - Familiar with software environment manager (modules)
  - Familiar with Veritas NetBackup software
  - Familiar with Sun Grid Engine (SGE) cluster queuing system

Research Assistant **May 2011 – December 2016**
SimCenter at the University of Tennessee at Chattanooga

Participant at ATPESC **July 31 – August 12 2016**
Attended the Argonne Training Program on Extreme-Scale Computing (ATPESC). ATPESC is a

Zhen HU

Ph.D., IEEE Member

Work History

- 08/2014 ~ present:
  Postdoctoral Fellow
  Department of Computer Science and Engineering
  College of Engineering and Computer Science
  University of Tennessee at Chattanooga, Chattanooga, Tennessee
- 04/2011 ~ 06/2013:
  Postdoctoral Research Associate
  The Center for Manufacturing Research
  College of Engineering
  Tennessee Technological University, Cookeville, Tennessee

Education

- 01/2007 ~ 12/2010:
  Doctor of Philosophy in Electrical and Computer Engineering
  Tennessee Technological University, Cookeville, Tennessee
  Dissertation: *Theory, Testbed and Optimization for Wireless Communication, Cognitive Radio, Cognitive Radar and Smart Grid*
- 09/2004 ~ 12/2006:
  Master's Degree in Communication and Information System
  Southeast University, Nanjing, China
  Thesis: *Studies in Dynamic Resource Allocation Algorithms for Multi-antenna System*
- 09/2000 ~ 06/2004:
  Bachelor's Degree in Electronics and Information Engineering
  Bachelor's Degree in Computer Science and Technology
  Huazhong University of Science & Technology, Wuhan, China

Research Experiences (2014 - Present)

- Perform innovative research on smart grid in terms of observability, controllability, and sustainability, which has contributed to one proposal, Collaborative Research: Robust Asset-and-User-Aware Dispatch of the Power Distribution Grid during Extreme Temperatures, funded by NSF in 2016.
- Perform novel research on connected & autonomous vehicles in terms of safety, efficiency, and scalability, which has contributed to one proposal, US Ignite: Collaborative Research: Focus Area 1: Fleet Management of Large-Scale Connected Autonomous Vehicles, funded by NSF in 2016.
- Perform comprehensive investigation on smart grid, smart building, smart health, environment surveillance, intelligent transportation, advanced wireless communications, and smart & connected communities, which has contributed to five research grants funded by Tennessee Higher Education Commission through Center for Excellence in Applied Computational Science & Engineering in 2015 and 2016.

- Response to precision medicine by investigating health care informatics and management; Improve post-stroke management efficiency and patient outcomes through multi-modal big data synthesis and analytics, which has contributed to one proposal submitted to NSF.
- Propose a fundamental research concept of health-centric urban mobility; Promote active transportation and mobility-on-demand/shared-ride public transportation; Foster cross-disciplinary collaborations between academic researchers and community stakeholders to build Chattanooga, TN as a model city for happy citizens with personalized, healthy, and environmentally-friendly mobility, which has contributed to one proposal submitted to NSF.

Selected Publications

- Jin Cho, **Zhen Hu**, Nancy Fell, Greg Heath, Rehan Qayyum, and Mina Sartipi, "Hospital Discharge Disposition of Stroke Patients in the State of Tennessee," resubmitted to *Southern Medical Journal*, 2017.
- Brian Williams, Brandon Allen, **Zhen Hu**, Hanna True, Jin Cho, Austin Harris, Nancy Fell and Mina Sartipi, "Real-Time Fall Risk Assessment Using Functional Reach Test," *International Journal of Telemedicine and Applications*, 2017.
- **Zhen Hu**, Salman Mohagheghi, and Mina Sartipi, "Efficient Data Acquisition in Advanced Metering Infrastructure," in IEEE PES General Meeting, Denver, CO, July 26-30, 2015.
- Jason Bonior, **Zhen Hu**, Terry N. Guo, Robert C. Qiu, James P. Browning, and Michael C. Wicks, "Software-Defined-Radio-Based Wireless Tomography: Experimental Demonstration and Verification," *IEEE Geoscience and Remote Sensing Letters*, vol. 12, no. 1, pp. 175 – 179, January, 2015.
- **Zhen Hu**, Shujie Hou, Michael C. Wicks, and Robert C. Qiu, "Wireless Tomography in Noisy Environments Using Machine Learning," *IEEE Transactions on Geoscience & Remote Sensing*, vol. 52, no. 2, pp. 956 – 966, February, 2014.

Farah Kandah

Department of Computer Science Engineering
University of Tennessee at Chattanooga
735 Vine Street
Chattanooga, TN 37405

a. Professional Preparation

• B. A. in Computer Science	The Hashemite University, Jordan, 2002
• M. S. in Computer Science	The University of Jordan, Jordan, 2005
• Ph. D. in Computer Science	North Dakota State University, Fargo, ND 2012

b. Appointments

• Assistant Professor University of Tennessee at Chattanooga	Department of Computer Science and Engineering Aug. 2012 – Present
• Teaching Assistant North Dakota State University	Department of Computer Science 2011 - 2012
• Research Assistant North Dakota State University	Department of Computer Science 2009 - 2011
• Lecturer and Course Coordinator The Hashemite University	Department of Computer Science 2005 - 2007
• Research Assistant The University of Jordan	Department of Computer Science 2003 - 2005

c.i. 5 Publications Most Closely related to the Proposed Project

1. Farah Kandah, and Jesse Whitehead: Trust-based Survivability Provisioning in Wireless Mesh Networks, *International Journal of Information Processing and Management (IJIPM 2016).*
2. Farah Kandah, and Jesse Whitehead: Energy-aware Multipath Provisioning in Wireless Mesh Networks, *Consumer Communications and Networking Conference (CCNC 2015).*
3. Farah Kandah, and Adrain Powell: Ultimate Control and Security Over Data Localization in the Cloud, *International Conference on Computing, Networking and Communications (ICNC 2015).*
4. Farah Kandah, Yashaswi Singh, Weiyi Zhang and Yulu Ma: Mitigating Misleading Routing Attack using Path Signature in Mobile Ad-Hoc Networks, *Global Communications Conference (GLOBECOM), 2013 IEEE*, pp.617-622, 2013.
5. Farah Kandah, Yashaswi Singh, and Weiyi Zhang: Mitigating Colluding Injected Attack using Monitoring Verification in Mobile Ad-hoc Networks, *Security and Communication Networks (SCN), Wiley*, 6, pp. 539-547, 2013.

c.ii. 5 Other Significant Publications

1. Farah Kandah, Yashaswi Singh, and Weiyi Zhang: Mitigating Eavesdropping Attack using Secure Key Management Scheme in Wireless Mesh Networks, *Journal of Communications*, 7, pp. 596-605, 2012.
2. Weiyi Zhang, Farah Kandah, Xiaojiang Du, and Chonggang Wang: Self-protecting Net- working using Dynamic p-cycle Consideration with Link Capacity Constraint, *Security and Communication Networks, Wiley*, 2011.
3. Farah Kandah, Yashaswi Singh, Weiyi Zhang, and Tie Wang: A Misleading Active Routing Attack in Mobile Ad-hoc Networks, *International Journal of Security and Networks (IJSN)*, 7, pp. 17-29, 2011.
4. Weiyi Zhang, Farah Kandah, Chonggang Wang, and Hongxiang Li: Dynamic Light Trail Routing in WDM Optical Networks, *Photonic Network Communications*, 21, pp. 7889, 2011.
5. Farah Kandah, Weiyi Zhang, Xiaojiang Du, and Yashaswi Singh: A Secure Key Manage- ment Scheme in Wireless Mesh Networks, *Communications (ICC), 2011 IEEE International Conference*

on, pp.1-5, 2011.

d. Synergistic Activities (up to 5)

1. IEEE Member and IEEE Communication Society (ComSoc) member.
2. Served on Technical Program Committee for IEEE WCNC 2013 - 2015, IEEE ICC 2015, IEEE/ACM ICCVE 2012 - 2015, and IEEE Globecom 2010 - 2013.
3. Journal Reviewer: WILEY's Security and Communication Networks (SCN) Journal, Inter- national Journal of Information Processing and Management (IJIPM), Journal of Computer Systems, Networks and Communications (JCSNC).
4. Guest Editor: IEEE Comsoc Multimedia Communications Technical Committee (MMTC), Special Issue on Multimedia Communications in Future Wireless Networks (E-letter).
5. ChinaCom2012: Network and Information Security Symposium CO-Chair.

HOPE KLUG
Department of Biology, Geology, & Environmental Science
University of Tennessee at Chattanooga
Dept. 2653, 615 McCallie Ave.
Chattanooga, TN 37403 USA

PROFESSIONAL PREPARATION

University of Florida	Zoology	Ph.D., 2007
University of Florida	Zoology and Psychology	B.S. with highest honors, 2001

APPOINTMENTS

University of Tennessee Chattanooga	UC Foundation Associate Professor	2016 - present
University of Tennessee Chattanooga	UC Foundation Assistant Professor	2015 - 2016
University of Tennessee Chattanooga	Assistant Professor	2011 - 2016
Yale University	Lab Associate Courtesy Appointment	2011 - 2012
Yale University	Post-Doctoral Associate	2010 - 2011
University of Helsinki	NSF Post-Doctoral Fellow	2008 - 2010

PUBLICATIONS

Five most relevant:

Reyes, E., Thrasher, P., Bonsall, M.B., and **Klug, H.** 2016. Population-level density dependence influences the origin and maintenance of parental care. PLOS ONE. DOI:10.1371/journal.pone.0153839

Klug, H., Bonsall, M.B., & Alonzo, S.H. 2013. The origin of parental care in relation to male and female life-history. Ecology & Evolution. 3:779-791.

Kokko, H., **Klug, H.**, & Jennions, M.D. 2012. Unifying cornerstones of sexual selection: operational sex ratio, Bateman gradient, and the scope for competitive investment. Ecology Letters (invited review). 15:1340-1351.

Klug, H. & Bonsall, M.B. 2010. Life history and the evolution of parental care. Evolution. 64:823-835.

Klug, H., Lindström, K., & Kokko, H. 2010. Who to include in measures of sexual selection is no trivial matter. Ecology Letters. 13:1094-1102.

Five additional publications:

Klug, H. 2014. Evolution: students debate the debate (Correspondence). Nature 515:343.

Klug, H., Alonzo, S.H., & Bonsall, M.B. 2012 "Theoretical foundations of parental care", in The Evolution of Parental Care (eds. Royle, N.J., Smiseth, P.T., Kölliker, M.). Oxford University Press.

Jennions, M.J., Kokko, H., & **Klug. H.** 2012. The opportunity to be misled in studies of sexual selection. Journal of Evolutionary Biology. 25:591-598.

Klug, H. & Bonsall, M.B. 2007. When to care for, abandon, or eat your offspring: the evolution of parental care and filial cannibalism. American Naturalist. 170: 886-901.

Klug, H., Lindström, K., & St. Mary, C. M. 2006. Parents benefit from eating offspring: density-dependent egg survivorship compensates for filial cannibalism. Evolution 60: 2087-2095.

SELECTION OF MAJOR GRANTS & FELLOWSHIPS

2016-2021	National Science Foundation, Division of Environmental Biology: CAREER: The operation of mate acquisition revisited ($655,000) (PI: H. Klug)
2016-2017	University of Tennessee at Chattanooga Engaged Grant: Developing a UTC-TN Aquarium Partnership ($20,000) (PI: H. Klug; Co-PIs: P. Foerder and A. Carroll)
2015-2016	Foundation of Greater Chattanooga Grant: Enrichment for students and animals: Using Animal Behavior to Encourage STEM Learning ($15,000) (PI: P. Foerder; Co-PIs: H. Klug & L. Hayes)

2013-2016	National Science Foundation: MRI: Acquisition of growth chambers for global change biology research and research training at the University of Tennessee at Chattanooga. NSF Division of Biological Infrastructure, Major Research Instrumentation. ($342,945) (PI: J. Boyd; Co-PIs: S. Chatzimanolis, H. Klug, J. Shaw, & T. Wilson)
2008-2010	National Science Foundation International Research Program: The Role of Resource Competition and Density Dependence in Sexual Selection Theory ($174, 362) (PI)
2006-2008	National Science Foundation Doctoral Dissertation Improvement Grant: The evolutionary significance of filial cannibalism in fishes with parental care ($12,000) (Co-PI with H. J. Brockmann)
2004-2007	National Science Foundation Graduate Research Fellowship ($102,000)
2003-2004	National Science Foundation GK-12 SPICE (Science Partners in Inquiry-based Collaborative Education, PI: D. Levey) Fellowship ($29,000)

SYNERGISTIC ACTIVITIES

1- Pre-collegiate Training & Outreach

Enrichment for students and animals: Using Animal Behavior to Encourage STEM Learning

I am co-leading an outreach project in which undergrad and K-12 students from a local all-female STEM school develop enrichment programs at the TN Aquarium, Chattanooga Zoo, & Nature Center.

GEAR UP & Girl Scout STEM Event, University of Tennessee Chattanooga:

For five years, I lead hands-on, inquiry-based science activities for 200+ middle and high school students through two local programs.

Science Education Outreach Program (SEOP), Yale University:

During Spring 2010, I participated in SEOP, an outreach program aimed to improve student's understanding of genetics and DNA and implemented hands-on activities in local middle schools.

Science Partners in Inquiry-Based Collaborative Education (SPICE), University of Florida:

During 2003 & 2004, I participated in SPICE, an NSF funded GK-12 program aimed at fostering inquiry-based education of science and math in students under-represented in these disciplines. As a participant in SPICE, I spent 9 months working with teachers & students in an under-resourced middle school, participated in curriculum development and mentored students.

Student Science Training Program (SSTP), University of Florida:

As a mentor in this program, I supervised 3 high school students for 7 weeks in my lab during the summers of 2003 & 2005. These students completed independent projects, gave formal presentations, and conducted published research (Klug et al. 2008).

2- Undergraduate Training

I have integrated undergraduates in all aspects of my research. I have supervised 55 undergraduates at the Universities of Tennessee at Chattanooga, Florida, and Helsinki and at Yale University. Several students have completed honors theses and five are coauthors on peer-reviewed manuscripts.

3- Graduate Student Research Training

I have supervised two M.S. in Environmental Science students, served as a Ph.D. Examiner for the Australian National University and Norwegian University of Science & Technology. I have served on the graduate committees of 12 additional students.

4- *Editorial board memberships:*

Proceedings of the Royal Society B (Associate Editor, 2013—ongoing)
Journal of Evolutionary Biology (Reviewing Editor, 2012—ongoing)

5- International Scholarship

I have made international collaboration and scholarship a priority. I have collaborated with scholars in Finland, Australia, the UK, & the US and presented my work in 11 countries (US, Finland, Canada, Brazil, France, Italy, UK, Australia, Sweden, Norway, China).

T. Daniel Loveless
Assistant Professor
Electrical Engineering Department
University of Tennessee at Chattanooga
Chattanooga, TN

a. Professional Preparation

Georgia Institute of Technology, Atlanta, GA, Electrical Engineering, B.S. 2004
Vanderbilt University, Nashville, TN, Electrical Engineering, M.S. 2007
Vanderbilt University, Nashville, TN, Electrical Engineering, Ph.D. 2009

b. Appointments

2014-present	Assistant Professor, Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, TN
2013-2014	Research Assistant Professor, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, TN
2011-2013	Adjunct Assistant Professor, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, TN
2009-2013	Senior Research Engineer, Institute for Space and Defense Electronics, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, TN
2009-2010	Instructor, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, TN

c. Products

Total number of publications: 82 (65 refereed articles/proceedings, 12 non-refereed proceedings, 2 theses, 3 book chapters)

Google Scholar **h-index of 17**; **i10-index of 31**; ≥ 909 total citations

Recent Publications (*Student Author)

1. **T. D. Loveless**, S. Jagannathan, E. X. Zhang, D. Fleetwood, J. Kauppila, L. W. Massengill, "Combined Effects of Total Ionizing Dose and Temperature on a K-band Quadrature LC-Tank VCO in a 32 nm CMOS SOI Technology," *IEEE Trans. Nucl. Sci.*, vol. PP, no. 99, pp. 1-1, Jan. 2017.
2. *Y. P. Chen, **T. D. Loveless**, A. L. Sternberg, E. X. Zhang, J. S. Kauppila, B. L. Bhuva, W. T. Holman, M. L. Alles, R. A. Reed, R. D. Schrimpf, D. McMorrow, and L. W. Massengill, "Persistent Laser-Induced Leakage in a 20 nm Charge-Pump Phase-Locked Loop (PLL)," *IEEE Trans. Nucl. Sci.*, vol. PP, no. 99, pp. 1-1, Jan. 2017.
3. *Y. P. Chen, L. W. Massengill, B. L. Bhuva, W. T. Holman, **T. D. Loveless**, W. H. Robinson, N. J. Gaspard, and A. F. Witulski, "Single-Event Characterization of Bang-Bang All-Digital Phase-Locked Loops (ADPLLs)," vol. 62, no. 6, pp. 2650-2656, Dec. 2015.
4. *K. J. Shetler, N. M. Atkinson, W. T. Holman, J. S. Kauppila, **T. D. Loveless**, A. F. Witulski, B. L. Bhuva, E. X. Zhang, and L. W. Massengill, "Radiation Hardening of Voltage References Using Chopper Stabilization," vol. 62, no. 6, pp. 3064-3071, Dec. 2015.
5. **Loveless, T. D.** and Holman, W. T. (2015). Single-Event Mitigation Techniques for Analog and Mixed-Signal Circuits. In. M. Bagatin & Gerardin (Eds.), *Ionizing Radiation Effects in Electronics: From Memories to Imagers* (Chp. 9).
6. J. S. Kauppila, L. W. Massengill, D. R. Ball, M. L. Alles, R. D. Schrimpf, **T. D. Loveless**, *J. Maharrey, *R. C. Quinn, J. D. Rowe, "Geometry-Aware Single-Event Enabled Compact Models for Sub-50 nm Partially Depleted Silicon-on-Insulator Technologies," *IEEE Trans. Nucl. Sci.*, vol. 62, no. 4, pp. 1589-1598, Aug. 2015.

7. T. D. Haeffner, **T. D. Loveless**, E. X. Zhang, A. L. Sternberg, *S. Jagannathan, R. D. Schrimpf, J. S. Kauppila, M. L. Alles, D. M. Fleetwood, L. W. Massengill, and N. F. Haddad, "Irradiation and Temperature Effects for a 32 nm RF Silicon-on-Insulator CMOS Process," *IEEE Trans. Nucl. Sci.*, vol. 61, no. 6, pp. 3037-3042, Dec. 2014.
8. *Y. P. Chen, **T. D. Loveless**, *P. Maillard, *N. J. Gaspard, *S. Jagannathan, A. L. Sternberg, E. X. Zhang, A. F. Witulski, B. L. Bhuva, W. T. Holman, and L. W. Massengill, "Single-Event Transient Induced Harmonic Errors in Digitally Controlled Ring Oscillators," *IEEE Trans. Nucl. Sci.*, vol. 61, no. 6, pp. 3163-3170, Dec. 2014.
9. *N. N. Mahatme, *N. J. Gaspard, *T. Assis, *I. Chatterjee, **T. D. Loveless**, B. L. Bhuva, W. H. Robinson, L. W. Massengill, S.-J. Wen, R. Wong, "Kernel-Based Circuit Partition Approach to Mitigate Combinational Logic Soft Errors," *IEEE Trans. Nucl. Sci.*, vol. 61, no. 6, pp. 3274-3281, Dec. 2014.

Recent Conference Proceedings (*Student Author)

10. *INVITED* "Hardening-By-Design Techniques for Analog and Mixed-Signal ASICs," by T. D. Loveless, presented at the 12th International School on the Effects of Radiation on Embedded Systems for Space Applications (SERESSA), Montreal, Quebec, Canada, Nov. 2016.
11. *INVITED* "Radiation Effects and Basic Mitigation Techniques for Mixed-Signal Electronics," by T. D. Loveless, presented at the 2016 Hardened Electronics and Radiation Technology (HEART) Conference, Monterey, CA, Apr. 2016.
12. *INVITED* "Hardening-By-Design Techniques for Analog and Mixed-Signal ASICs," by T. D. Loveless, presented at the 11th International School on the Effects of Radiation on Embedded Systems for Space Applications (SERESSA), Puebla, Mexico, Dec. 2015.

d. Activities

1. Project mentor for nine 11th grade students from the STEM High School Fab Lab, "Mitigating Cold-Temperature Effects in High-Altitude Balloon Payloads," Oct.-Dec. 2016.
2. Panelist, The Baylor School Accelerator's Entrepreneurial Panel, "How to Develop an Idea," Nov. 2016.
3. "The Martian" and "UTChattSat: Engineering for Outer Space in the Classroom," Outreach Presentations at the Chattanooga Girls Leadership Academy, Chattanooga, TN, Apr. 19, 2016 and Oct. 6, 2016.
4. Recipient of 2016 GigTank365 Summer Fellowship (UTChattSat), *Co.Lab*, Chattanooga, TN, May-July 2016.
5. STEM Category Winner in Faculty Elevator Speech Competition, "Rocket Scientist, Engineer, Educator," *UTC's Research Dialogues*, Apr. 2016.
6. Outstanding Researcher Award, Electrical Engineering, University of Tennessee at Chattanooga, 2015-2016.
7. UTC General Education Steering Committee, Jan. 2017-present.
8. Awards committee, 2016 IEEE Nuclear and Space Radiation Effects Conference, May-Sept., 2016.
9. "Minimum Size and Maximum Packing Density of Nonredundant Semiconductor Devices," Baylor School Journal Club, Feb. 21, 2016.
10. Led the Electrical Engineering Department's efforts in 2015-2016 ABET re-accreditation cycle. Established college-wide methodology for student outcome assessment, Nov. 2015.
11. Community liaison for the College of Engineering and Computer Science (CECS) Electrical Engineering Department, Oct. 2015-present.
12. Member of the UTC Departmental Honors Committee, Sept. 2015-Aug. 2016.
13. Elevated to Senior Member, IEEE, June 2015.
14. Mentor for one East Ridge High School Senior project in electrical engineering, Jan.-May 2015.
15. Recipient of 3 best paper awards: GOMACTech 2012, IRPS 2011, GOMACTech 2010.
16. Recipient of the 2008 IEEE Nuclear Plasma and Sciences Society (NPSS) Graduate Scholarship Award for contributions to the fields of Nuclear and Plasma Sciences, March 2008.

Soubantika Palchoudhury, Ph.D.

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Chemical Engineering
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Tel: (423) 425-5455, Email: soubantika-palchoudhury@utc.edu

Education

Ph.D. **The University of Alabama**, Chemical Engineering, Tuscaloosa, Alabama, 2012
Dissertation: Synthesis and Characterization of Platinum Decorated Iron Oxide Nanoparticles for Biomedical Applications
M.S. **The University of Alabama**, Chemical Engineering, Tuscaloosa, Alabama, 2010
B.S. **National Institute of Technology, Durgapur**, Chemical Engineering, India, 2008

Academic Experience

- **University of Tennessee at Chattanooga**, Visiting Assistant Professor, Aug 2015-Present
- **The University of Alabama,** Center for Materials and Information Technology (MINT) Tuscaloosa, Alabama, Postdoctoral Researcher, Feb 2014-Aug 2015
- **University of South Carolina,** Arnold School of Public Health, Columbia, South Carolina, Postdoctoral Researcher, June 2013-Feb 2014
- **Yale University**, Chemical and Environmental Engineering, New Haven, Connecticut, Postdoctoral Researcher, June 2012-June 2013

Current Membership in Professional Organizations

American Institute of Chemical Engineers, American Chemical Society, and Royal Society of Chemistry

Selected Honors, Awards, and Grants

- Center for Integrated Nanotechnologies (CINT) User Proposal Award, LANL (2016)
- Provost Student Research Award UTC (Student: Megan Downs), UTC (2016), $ 1000.00
- TBAEE Laboratory Equipment Grant for Chemical Eng., UTC (2015), Co-PI, $ 26,761.00

Editorial Board and Peer-Review Experience

Editorial Board Member: Int. J. Measurement Technol. Instrumen. Eng.
JAP/APL, Nanomaterials, Yale J Biol Med, Langmuir, ES&T, Nanoscale, INJP, Dovepress, J En Storage

Selected Publications

Publication: 21, Book chapters: 4, Highlight in Nature: 1, Cover art: 1, h-index: 11, Citations ~ 401

1. ***Palchoudhury, S.;*** Zhou, Z.; Ramasamy, K.; Okirie, F.; Prevelige, P.; Gupta, A. "Self-Assembly of P22 Protein Cages with Iron Oxide Nanoparticles and Polyamidoamine Dendrimers" JMR (2016, **Invited Paper, communicating author**)
2. ***Palchoudhury, S.;*** Ramasamy, K.; Gupta, A. "Recent Progress in Spintronic Materials" Material Matter. (2016, **Invited Paper**)
3. Ghosh, A; ***Palchoudhury, S.;*** Thangavel, R.; Zhou, Z.; Naghibolashrafi, N.; Ramasamy, K.; Gupta, A. "A New Family of Wurtzite-Phase Cu_2ZnAS_{4-x} and $CuZn_2AS_4$ (A= Al, Ga, In) Nanocrystals for Solar Energy Conversion Applications" ChemComm (2015, **Cover art, communicating author**)
4. ***Palchoudhury, S.;*** Palchaudhuri, S. "Rapid Determination of Hexavalent Chromium in ppb Level and Speciation of the Metal with a New Organic Reagent, Bis(pyrrole-2aldehydo)thiocarbohydrazone (BPATCH) in Presence of Vanadium(V)" J. Indian Chem. Soc. (2016)

5. ***Palchoudhury, S.;*** Lead, J.R. "A Facile and Cost-Effective Method for Separation of Oil-Water Mixtures using Polymer-Coated Iron Oxide Nanoparticles" Env. Sci. Technol. (2014)
6. ***Palchoudhury, S.;*** Hyder, F.; Vanderlick, K; Geerts, N. "Water-Soluble Anisotropic Iron Oxide Nanoparticles: Dextran-Coated Crystalline Nanoplates and Nanoflowers" Part. Sci. &Technol. (2013)
7. ***Palchoudhury, S.;*** Xu, Y.; Rushdie, A.; Holler, R.; Bao, Y. "Controlled Synthesis of Iron Oxide Nanoplates and Nanoflowers" ChemComm (2012)
8. ***Palchoudhury, S.;*** Xu, Y.; Rushdie, A.; Bao, Y. "DNA Interaction of Platinum Attached Iron Oxide Nanoparticles" IEEE Transactions (2012)
9. ***Palchoudhury, S.;*** An, W.; Xu, Y.; Qin, Y.; Zhang, Z.; Holler, R.; Turner, C. Heath; Chopra, N.; Bao, Y. "Synthesis and Growth Mechanism of Iron Oxide Nanowhiskers" Nano Lett. (2011). **First paper to report maghemite nanowhiskers by this method.**
10. ***Palchoudhury, S.;*** Xu, Y.; Goodwin, J.; Bao, Y. "Synthesis of Multiple Platinum Attached Iron Oxide Nanoparticles" J. Mater. Chem. (2011)
11. ***Palchoudhury, S.;*** Xu, Y.; Goodwin, J.; Bao, Y. "Synthesis of Iron Oxide Nanoworms" J. Appl. Phys. (2011)
12. ***Palchoudhury, S.;*** Xu, Y.; An, Wei; Turner, C. H.; Bao, Y. "Platinum Attachments on Iron Oxide Nanoparticle Surfaces" J. Appl. Phys. (2010)
13. Gupta, R; Candler, J.; ***Palchoudhury, S.;*** Ramasamy, K.; Gupta, B. "Flexible and High Performance Supercapacitors based on $NiCo_2O_4$ for Wide Temperature Range Applications" Sci. Rep. (2015)
14. Ramasamy, K.; Gupta, R.; ***Palchoudhury, S.;*** Ivanov, S.; Gupta, A. "Layer-Structured Copper Antimony Chacogenides ($CuSbSe_xS_{2-x}$): Stable Electrode Materials for Supercapacitors" Chem. Mater. (2014)
15. Li, H.; Melnyczuk, J.; Lauchon, L.; ***Palchoudhury, S.;*** Wu, J.; Nagappan, P.; Harruna, I.; Wang, X. "Selectively Self-assembling Graphene Nanoribbons with Shaped Iron Oxide Nanoparticles" RSC Adv. (2014)
16. Xu, Y.; ***Palchoudhury, S.;*** Yin, Q.; Macher, T.; Bao, Y. "Make Conjugation Simple: A Facile Approach to Integrated Nanostructures" Langmuir. (2012)
17. Xu, Y.; Yin, Q.; ***Palchoudhury, S.;*** Bao, Y. "Water Soluble Iron Oxide Nanoparticles with High Stability and Selective Surface Functionality" Langmuir. (2011). **Highlight in Nature.**
18. Sikder, J.; Pereira, C.; ***Palchoudhury, S.;*** Vohra, K.; Basumatary, D.; Pal, P. " Synthesis and Characterization of Cellulose acetate-polysulfone Blend Microfiltration Membrane for Separation of Microbial Cells from Lactic Acid Fermentation Broth" Desalination (2009)
19. **Book Chp.**: Ramasamy, K.; ***Palchoudhury, S.;*** Gupta, A. "Synthesis and Properties of Magnetic Chalcogenide Nanostructures", Wiley (2016, Accepted)
20. **Book Chp.**: Melnyczuk, J; ***Palchoudhury, S.*** "Introduction to Bio-Inspired Hydrogel and Their Applications", Emerging Research on Bioinspired Materials Engineering (2016)
21. **Book Chp.**: ***Palchoudhury, S.;*** Baalousha, M.; Lead, J.R. "Methods for Measuring Concentration of Nanoparticles", Frontiers in Nanoscience. (2015)
22. **Book Chp.**: Melnyczuk, J; ***Palchoudhury, S.*** "Synthesis and Characterization of Iron Oxide Nanoparticles", Handbook of Research on Nanoscience, Nanotechnol. & Adv Mater. (2014)

Selected Posters & Presentations

1. ***Palchoudhury, S.*** "Synthesis and Characterization of Hybrid Nanoparticles for Biomedical and Environmental Remediation Applications", International Conference and Exhibition on Materials Science and Engineering, 13th Sep 2016 (Invited talk)
2. ***Palchoudhury, S.*** *et al.*; "Self-Assembly of Protein Cages with Polymer and Nanoparticles", NanoBio Summit, 23rd Oct 2014
3. ***Palchoudhury, S.*** "Synthesis and Characterization of Nanostructures for Biomedical Applications", Sammilani College, India, 21st Dec 2012 (Invited talk)
4. ***Palchoudhury, S.***; Xu, Y.; Bao, Y. "Synthesis of Multiple Platinum Attached Iron Oxide Nanoparticles", 140th TMS Conference, 2nd Mar 2011

Hong Qin
University of Tennessee at Chattanooga
Dept of Computer Science & Engineering, Dept of Biology, Geology & Environ. Sci., SimCenter
Phone: 423-425-4329 Fax: 423-425-5442 Email: hong-qin@utc.edu

a. Professional Preparation

- Tsinghua University, China, Biological Sciences and Biotechnology, B.S, 1991
- Tsinghua University, China, Biophysics, M.S.,1994
- University of Chicago, Biochemistry and Molecular Biology, Ph.D, 2000
- Loyola University of Chicago, Computer Science, M.S., 2002

b. Appointments

- Associate Professor, joint appointment of Dept of Computer Science & Engineering and Dept of Biology, Geology & Environmental Science, August 2016 – present.
- Associate Professor, Dept of Biology, Spelman College, September 2015 – July 2016.
- Assistant Professor, Dept of Biology, Spelman College, August 2009 – August 2015.
- Assistant Professor, Dept of Agricultural and Environmental Sciences, and Dept of Biology, Tuskegee University, February 2007 – July 2009.
- Research Assistant Professor, Department of Biostatistics and Computational Biology, Center for Aging and Development Biology, University of Rochester. January 2004- June 2006

c. Publications (10 out 20)

i) Five publications most closely related to proposed project:

- Guven, E., L.A. Parnell, E.D. Jackson, M.C. Parker, N. Gupta, J. Rodrigues, and H. Qin, Hydrogen peroxide induced loss of heterozygosity correlates with replicative lifespan and mitotic asymmetry in Saccharomyces cerevisiae. PeerJ, 2016. 4: p. e2671
- Jiang*, Y., H. Qin*, and L. Yang, *Using network clustering to predict copy number variations associated with health disparities.* PeerJ, 2015. 3: p. e677.4358638. (*co-first authors).
- Qin, H. and A. Driks, *Contrasting evolutionary patterns of spore coat proteins in two Bacillus species groups are linked to a difference in cellular structure.* BMC Evol Biol, 2013. 13(1): p. 261.
- Qin, H. and L. Yang, *Detection of changes in transitive associations by shortest-path analysis of protein interaction networks integrated with gene expression profiles.* Proceedings of the IEEE International Conference on Biomedical Engineering and Informatics, 2008. **1**: p. 418-423.
- Qin, H., *Teaching computational thinking through bioinformatics to biology students.* Proceedings of 40th ACM Technical Symposium on Computer Science Education, 2009: p. 188-191.

ii) Five other significant publications:

- Guo, Z., A.B. Adomas, E.D. Jackson, H. Qin, and J.P. Townsend, *SIR2 and other genes are abundantly expressed in long-lived natural segregants for replicative aging of the budding yeast Saccharomyces cerevisiae.* FEMS Yeast Res, 2011. **11**(4): p. 345-55.
- Qin, H., M. Lu, and D.S. Goldfarb, *Genomic instability is associated with natural life span variation in Saccharomyces cerevisiae.* PLoS ONE, 2008. **3**(7): p. e2670.
- Qin, H., H.H. Lu, W.B. Wu, and W.H. Li, *Evolution of the yeast protein interaction network.* Proc Natl Acad Sci U S A, 2003. **100**(22): p. 12820-4.
- Gilchrist, M.A., H. Qin, and R. Zaretzki, *Modeling SAGE tag formation and its effects on*

data interpretation within a Bayesian framework. BMC Bioinformatics, 2007. **8**: p. 403.
- Qin, H., W.B. Wu, J.M. Comeron, M. Kreitman, and W.H. Li, *Intragenic spatial patterns of codon usage bias in prokaryotic and eukaryotic genomes*. Genetics, 2004. **168**(4): p. 2245-60.

d. Synergistic Activities

- **UTC SimCenter.** Qin is a member of the SimCenter, a Center of Excellence in Applied Computational Science and Engineering http://www.utc.edu/college-engineering-computer-science/research-centers/simcenter/. Qin leads the Health and Biosystems program at SimCenter.

- **NSF CAREER award** #1453078, "A probabilistic gene network model of cellular aging and its application on the conserved lifespan extension mechanisms of dietary restriction". Qin is a recipient of NSF CAREER ward for his research on mathematic modeling of cellular aging and development of computational tools for studies on aging.

- **Faculty Mentor Fellow of Quantitative Undergraduate Biology Education and Synthesis (QUBES)**: Qin is a inauguration member of QUBES Faculty Mentor Fellow in 2017. Qin leads a regular online faculty workshop on integrating computing into undergraduate interdisciplinary education and research.

- **Quantitative Biology Community**: Qin is a co-organizer a workshop series, "Finding your inner modeler: how computational biology can advance your research and how to get started", supported by an NSF MCB award (PI David Stone, U of Illinois at Chicago). Qin also recently co-organized an NSF-sponsored workshop "A strategic planning workshop to explore quantitative biology as a vehicle for broad participation" (see https://youtu.be/eoQ0VXcSimg)

- **YouTube Educational Channel**, http://youtube.com/c/hongqin. Qin has been developing educational and tutorial videos since 2009. His educational channel covers computational biology, molecular biology, and microbiology. His educational channel has over 400 subscribers and over 200,000 views. Qin's popular education videos include: "Visualizing protein structure in Swiss PDB Viewer", "How to use R match() function to merge different data sets", "Retrieve and analyze a gene expression data set from NCBI GEO in R", "Covert Excel file to csv and read into R", "Principle of site-directed mutagenesis by PCR" , "BD FACS Calibur, Cell Quest Training", "Hierarchical clustering by hclust in R on a distance matrix", "PCR product analysis followed by restriction enzyme analysis, ApE".

- **Open Science and Reproducible Research**, https://github.com/hongqin and https://github.com/QinLab. Qin is active in the open science community and support reproducible research initiative. Qin and members in his research group have been publically depositing codes and data of research projects in his lab at their GitHub sites.

Donald R. Reising
Assistant Professor
Electrical Engineering Department
University of Tennessee at Chattanooga
Chattanooga, TN

a. Professional Preparation

University of Cincinnati, Cincinnati, OH, Electrical Engineering, B.S. 2006
Air Force Institute of Technology, Dayton, OH, Electrical Engineering, M.S. 2009
Air Force Institute of Technology, Dayton, OH, Electrical Engineering, Ph.D. 2012

b. Appointments

2014-present	Assistant Professor, Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, TN
2009-2014	Electronics Engineer, Air Force Research Laboratory - Sensors Directorate, U.S. Air Force, Dayton, OH
2012-2014	Adjunct Assistant Professor, Department of Electrical and Computer Engineering, Air Force Institute of Technology, Dayton, OH
2009-2012	Research Associate, Department of Electrical and Computer Engineering, Air Force Institute of Technology, Dayton, OH
2006-2009	Electronics Engineer, Aeronautical Systems Center, U.S. Air Force, Dayton, OH

c. Products

(i) 5 Most closely related to Proposed Project (*Student Author)

1. *Wheeler and Reising, "Assessment of the Impact of CFO on RF-DNA Fingerprint Classification Performance". IEEE Int'l Conference on Computing, Networking and Communications (ICNC), Jan. 2017.
2. Reising, Temple, and Jackson, "Discriminating Authorized and Rogue Devices in an OFDM-Based Network Using Dimensionally Reduced RF-DNA Fingerprints," IEEE Trans on Information Forensics and Security, Vol. 10, No. 6, pp. 1180-1192, Jun. 2015.
3. Reising, Prentice, and Temple, "An FPGA Implementation of Real-Time RF-DNA Fingerprinting for RFINT Applications." 2011 Military Communications Conference (MILCOM 2011), Oct. 2011.
4. *Reising, Temple, and Mendenhall, "Improving Intra-Cellular Security Using Air Monitoring with RF Fingerprints," IEEE Wireless Communication and Networking Conference (WCNC), Apr. 2010.
5. *Reising, Temple, and Mendenhall, "Improved Wireless Security for GMSK-based Devices Using RF Fingerprinting," Int'l J. Electronic Security and Digital Forensics, Vol. 3, No. 1, pp. 41-59, 2010.

(ii) 5 Other Significant Products (*Student Author)

1. *Harmer, *Reising, and Temple, "Classifier Performance Comparison Using 2D RF-DNA Features". IEEE Int'l Conference on Communications (ICC), Jun. 2013.
2. *Reising, and Temple, "WiMAX Mobile Subscriber Verification Using Gabor-Based RF-DNA Fingerprints," IEEE Int'l Conference on Communications (ICC), Jun. 2012.

3. *Reising, Temple, and Oxley, "Gabor-based RF-DNA Fingerprinting for Classifying 802.16e WiMAX Mobile Subscribers," IEEE Int'l Conference on Computing, Networking and Communications (ICNC), Jan. 2012.
4. *Williams, Temple, and Reising, "Augmenting Bit-Level Network Security Using Physical Layer RF-DNA Fingerprinting," IEEE Global Communications Conference (GLOBECOM), Dec. 2010.

d. Activities

1. Reviewer for the Institution of Engineering and Technology (IET) Communications Journal, IEEE Military Communications (MILCOM) Conference, IEEE Symposium on Wireless Technology and Applications, IEEE Global Communications Conference, IEEE Transactions on Information Forensics and Security, IEEE Journal on Selected Areas in Communications, IEEE Asia-Pacific Conference on Applied Electromagnetics, and International Journal on Security and Communication Networks.
2. Faculty volunteer for UTC's Read2Achieve program for incoming freshman, 2015-present.
3. Faculty advisor for the Electrical Engineering Department Senior Design Course, 2015-present.
4. Faculty lead and coordinator for UTC's College of Engineering and Computer Science MakerSpace, 2015-present.

Mina Sartipi, PhD

UC Foundation Professor
Department of Computer Science and Engineering
The University of Tennessee at Chattanooga
Phone: (423) 425-5336, Fax: (423) 425-5442
Email: mina-sartipi@utc.edu

A. Professional Preparation

Sharif University of Technology	Tehran, Iran	Electrical Engineering	B.Sc., 2000
Georgia Institute of Technology	Atlanta, GA	Electrical and Computer Eng.	M.S., 2003
Georgia Institute of Technology	Atlanta, GA	Electrical and Computer Eng.	Ph.D., 2006

B. Appointments

2016–present **Urban Science and Technology Program Leader**
University of Tennessee at Chattanooga,
Chattanooga, TN, USA

2015–present **Professor & PhD Program Coordinator**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering,
Chattanooga, TN, USA

2011–2015 **Associate Professor**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering
Chattanooga, TN, USA

2007–2011 **Assistant Professor**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering
Chattanooga, TN, USA

2006–2007 **Assistant Professor**
University of Tennessee at Chattanooga, Dept. of Electrical Engineering
Chattanooga, TN, USA

C. Products

Products Most Closely Related to Proposal

[1] B. Williams, B. Allen, Z. Hu, H. True, J. Cho, A. Harris, N. Fell, and M. Sartipi, "Real-Time Fall Risk Assessment Using Functional Reach Test," The International Journal of Telemedicine and Applications, January 2017.

[2] Z. Hu, S. Mohagheghi, and M. Sartipi, "Efficient Data Acquisition in Advanced Meter Infrastructure", in Proc. of IEEE Power and Energy Society, July 2015.

[3] A. Harris, H. True, Z. Hu, J. Cho, N. Fell, and M. Sartipi, "Fall Recognition using Wearable Technologies and Machine Learning Algorithms," in the Proc. of IEEE Big Data Conference, December 2016.

[4] B. Williams, B. Allen, H. True, N. Fell, D. Levine, and M. Sartipi, "A Real-time, Mobile Timed Up and Go System", in Proc. of IEEE Body Sensor Networks Conference, June 2015.

[5] Z. Hu, S. Mohagheghi, and M. Sartipi, "Flexible Data Acquisition, Compression, and Reconstruction in Advanced Metering Infrastructure," in Proc. of Power Systems Conference, March 2016.

Other Significant Products

[1] J. Cho, Z. Hu, and M. Sartipi, "Post-stroke Discharge Disposition Prediction using Deep Learning," in Proc. of IEEE SoutheastCon, March 2017.

[2] B. Allen, R. Derveloy, N. Fell, W. Gasior, G. Yu, and M. Sartipi, "Telemedicine Assessment of Fall Risk Using Wireless Sensors," in Proc. of IEEE International Conference on Sensor and Ad Hoc Communications and Networks, June 2014.
[3] L. Yang, M. Sartipi, M. McNeely, "Usable Protection to Healthcare Application", in Proc. of ACM Workshop on Cyber Security and Information Intelligence Research, January 2011.
[4] F. Delgosha, M. Sartipi, and F. Fekri, "Construction of Two-dimensional Paraunitary Filter Banks over Fields of Characteristic Two and their Connections to Error-Control Coding," IEEE Transactions on Circuits and Systems I, Volume 55, Issue 10, pp. 3095-53109, November 2008.
[5] M. Sartipi, "LDPC Codes for Information Embedding and Lossy Distributed Source Coding", Proc. of IEEE Data Compression Conference, April 2010.

D. Synergistic Activities

- **IEEE Senior Member**
- **Founding Director**
  2012-present, Smart Communications and Analysis Lab
- **Mentoring of Young Women**
  As a female faculty member in the Computer Science and Engineering department, I encourage and advise undergraduate and graduate female students on research and possible careers in science.
- **Faculty Advisor for Computer Science Female Group**
  2016-present, Girls in Computer Science (GiCS)
- **Professional Services**
  - Presenter at multiple federal funding agency workshops
  - Keynote Speaker, Mid SouthEast ACM Conference
  - Planning member of the South Big Data Hub - Mobile Health
  - TPC member: Wireless / Radio Access Technologies VTC; International Workshop on Cyber-Physical System (CPS) and Its Computing and Networking Design at ICNC; IEEE GLOBECOM-Wireless Communications and Networking
  - Journal Reviewer: IEEE Transactions on Information Theory, IEEE Transactions on Communications, IEEE Communications Letters, IEEE Transactions on Signal Processing, EURASIP Journal on Wireless Communications and Networking
  - Conference Reviewer: IEEE INFOCOM, IEEE GLOBECOM, IEEE ISIT, IEEE ICC, IEEE SECON, IEEE ICASSP
- **Award**
  - UTC Outstanding Faculty Research and Creative Achievement award, 2016
  - "Keep the Stars Shining" Award, 2012
  - Outstanding Researcher in the College of Engineering and Computer Science, 2010, 2014, 2015
  - Outstanding Researcher in the Department of Computer Science and Engineering, 2010, 2013, 2015
  - Named UC Foundation Assistant Professor, 2008

KIDAMBI SREENIVAS
Associate Professor
Department of Mechanical Engineering
University of Tennessee at Chattanooga
Chattanooga, TN 37403

A. Professional Preparation:

Indian Institute of Technology, Madras, India	Aerospace Engineering	B.Tech.	1991
Mississippi State University	Aerospace Engineering	M.S.	1993
Mississippi State University	Engineering	Ph.D.	1996

B. Appointments:

2017 – Present	Associate Professor University of Tennessee at Chattanooga
2014 – Present	Joint Faculty Appointment Oak Ridge National Laboratory
2011 – Present	Research Professor University of Tennessee at Chattanooga
2002 – 2011	Associate Research Professor University of Tennessee at Chattanooga
2002 – 2002	Associate Research Professor Mississippi State University
1999 – 2002	Assistant Research Professor Mississippi State University
1998 - 1999	Visiting Researcher (Unstructured Grid Technology) Mississippi State University
1997 – 1998	Post-doctoral Fellow (Computational Fluid Dynamics) Mississippi State University
1991 – 1996	Graduate Research Assistant NSF ERC for Computational Field Simulation, Mississippi State University

C. 5 Publications Most Closely related to the Proposed Project:

1. Sreenivas, K., Webster, R., and Collao, D. M., "Computational Simulations of the Low-Noise SDT2-R4 Configuration Using Tenasi," AIAA Paper 2018-4203, Atlanta, GA, June 2018.
2. Tanis, C., Sreenivas, K., Newman, J.C., and Webster, R.S., "Performance Portability of a Multiphysics Finite Element Code," AIAA Paper 2018-2890, Atlanta, GA, June 2018.
3. Sreenivas, K., Mittal, A., Hereth, L., Taylor, L.K., and Hilbert, C.B., "Numerical Simulation of the Interaction between Wind Turbines," Journal of Wind Engineering and Industrial Aerodynamics, Vol. 157, pp 145-157, October 2016.
4. Azarnoosh, J., Sreenivas, K., Arabshahi, A., "CFD Investigation of Human Tidal Breathing through Human Airway Geometry," Procedia Computer Science, Vol. 80, 2016, pp 965 - 976.

1. for Wind Turbines," Journal of Computational Physics (accepted), available online 19 October, 2016.

A. 5 Other Significant Publications:

1. Mittal, A., Sreenivas, K., Taylor, L.K., Hereth. L., and Hilbert, C.B., "Blade-Resolved Simulations of a Model Wind Turbine: Effect of Temporal Convergence," Wind Energy, Vol. 19, Issue 10, pp 1761 – 1783, October 2016.
2. Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Numerical Simulation of Airflow in a CT-based Human Airway Model with Physiologically Appropriate Boundary Conditions," Poster Presentation within the Respiratory Bioengineering Track, Biomedical Engineering Society Annual Meeting, San Antonio, Texas, October 2014.
3. Hyams, D.G., Sreenivas, K., Pankajakshan, R., Nichols, III, D.S., Briley, W.R., and Whitfield, D.L., "Computational simulation of model and full scale Class 8 trucks with drag reduction devices," *Computers & Fluids*, Volume 41, Issue 1, February 2011, Pages 27-40.
4. Nichols, S., Sreenivas, K., Karman, S., and Mitchell, B., "Turbulence Modeling for Highly Separated Flows," *AIAA Paper 2007-1407*, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
5. Nichols, S., Mitchell, B., Sreenivas, K., Taylor, L., Whitfield D., and Briley, R., "Aerosol Propagation in an Urban Environment," *AIAA Paper 2006-3726*, June 2006.

B. Synergistic Activities (up to 5):

- SimCenter leadership role in unsteady viscous flow engineering applications, scientific computing, and unstructured grid technologies, including software development, integration, and management, and also facilitating teamwork to solve complex real-world engineering problems (University of Tennessee at Chattanooga)
- Thesis Advisor for 1 Ph.D. students (University of Tennessee at Chattanooga)
- Mentor for 3 honors students and three undergraduate student researchers (University of Tennessee at Chattanooga)
- Faculty advisor for the Flying Mocs, a student organization dedicated to pursuing the objectives of the AIAA design, build, fly competition

A. Collaborators and Co-Editors:

Mina Sartipi	University of Tennessee at Chattanooga
James Newman	University of Tennessee at Chattanooga
Robert Webster	University of Tennessee at Chattanooga
Craig Tanis	University of Tennessee at Chattanooga
Trevor Elliot	University of Tennessee at Chattanooga
Chuck Margraves	University of Tennessee at Chattanooga
Sungwoo Yang	University of Tennessee at Chattanooga
Abi Arabshahi	University of Tennessee at Chattanooga
Ethan Hereth	University of Tennessee at Chattanooga
Josh Epstein	NYU
Amar Singh	Erlanger Health System

Craig Tanis, PhD

craig-tanis@utc.edu
(423) 402-0226

Assistant Professor
University of Tennessee at Chattanooga
Department of Computer Science

Education

PhD Computational Engineering, University of Tennessee at Chattanooga, 2013

M.S. Computer Science, Tulane University, 1998

B.S.E. Computer Engineering, Tulane University, 1997

Publications

Citation Distance: Measuring Changes in Scientific Search Strategies. R. Whalen, Y. Huang, C. Tanis, A. Sawant, B. Uzzi, N. Contractor. *BigScholar, ACM WWW 2016*

Petrov-Galerkin and discontinuous-Galerkin methods for time-domain and frequency-domain electromagnetic simulations. W. K. Anderson, L. Wang, S. Kapadia, C. Tanis, and B. Hilbert. *Journal of Computational Physics, vol. 230, no. 23, Sep. 2011.*

Distributed Map-making Using Online Generalized Voronoi Graphs. J. Jennings, C. Kirkwood-Watts, C. Tanis. *Proceedings of the Conference on Automated Learning and Discovery (CONALD 98)*

Cooperative Localization and Map-making for Mobile Robots. C. Tanis *Tulane University Technical Report, May 1997.*

Presentations

Campus Champion Fellows *XSEDE 2016*

Lazy Evaluation of Unstructured Mesh Queries in C++ *ACM Mid-Southeast Conference, 2015*

Parallel Mesh Management Using PLatt (Poster) *SIAM PP12*

Professional Affiliations

ACM SIGHPC, SIGHPCEDUCATION. Member, 2014 - Present

XSEDE Campus Champions. Champion for UTC, 2014-Present

Upsilon Pi Epsilon. Member, 1997 - Present

Craig Tanis, PhD

Recognition

XSEDE Campus Champion Fellow 2015-16

2014 UTC Computer Science Teacher of the Year

2013 UTC Computer Science Teacher of the Year

2012 UTC Computer Science Teacher of the Year

Employment

University of Tennessee at Chattanooga – Assistant Professor, Computer Science, 2014 - Present

University of Tennessee at Chattanooga – Lecturer, Computer Science, 2010 - 2013

UTC SimCenter – Graduate Research Assistant, 2007-2010

Tanis Tech LLC – Consultant / Developer, 2006-2010

Advance Internet – Senior Programmer, 1999-2006

Johns Hopkins Applied Physics Lab – Professional Associate, 1998-1999

Tulane University – Graduate Research/Teaching Assistant, 1996-1998

Revised: 26 Jan 2017

Endong Wang, Ph.D., CPC, AIC, ASCE

Department of Engineering Management & Technology, EMCS 326B, University of Tennessee-Chattanooga, Chattanooga, TN 37403, Tel: 423-425-5778; Fax: 423-425-5818;
Email: Endong-Wang@utc.edu

Professional Preparation

Nanjing University of Science & Technology (Nanjing, China)	Structure Engineering	B.E.	2003
Southeast University (Nanjing, China)	Management Science	M.S.	2006
University of Nebraska-Lincoln (Lincoln, NE)	Construction	M.S.	2011
University of Nebraska-Lincoln (Lincoln, NE)	Engineering	Ph.D.	2013
University of Wisconsin-Milwaukee (Milwaukee, WI)	Sustainable Manufacturing	Postdoctoral	2013-2013

Appointments

2013–Present	Assistant Professor, Graduate Faculty, Construction Management, University of Tennessee-Chattanooga (UTC)
2013–2013	Postdoctoral Research Associate, Mechanical Engineering, University of Wisconsin-Milwaukee (UWM)
2009–2013	Graduate Research Assistant, Construction Management, University of Nebraska-Lincoln (UNL)
2008–2009	Adjunct Researcher, Key Laboratory of Contemporary Management Informatics
2006–2009	Instructor, Civil Engineering, Ocean University of China

Products

Five Products Most Closely Related to the Proposed Project

1. **Wang, E.**, Yuan, C. (2014). A hybrid life cycle assessment of atomic layer deposition process. Journal of Cleaner Production, 74, 145-154.
2. **Wang, E.**, Shen, Z. (2013). Lifecycle energy consumption prediction of residential buildings by incorporating longitudinal uncertainties. Journal of Civil Engineering and Management, 19, 161-171.
3. **Wang, E.**, Shen, Z. (2013). A hybrid Data Quality Indicator and statistical method for improving uncertainty analysis in LCA of complex system– application to the whole-building embodied energy analysis. Journal of Cleaner Production, 43,166-173.
4. **Wang, E.**, Shen, Z., Neal, J., Shi, J., Berryman, C., Schwer, A. (2012). An AHP-weighted aggregated data quality indicator (AWADQI) approach for estimating embodied energy of building materials. International Journal of Life Cycle Assessment, 17, 764-773.
5. Yuan, C., **Wang, E.**, Zhai, Q., Yang, F. (2015).Temporal discounting in life cycle assessment: A critical review and theoretical framework. Environmental Impact Assessment Review, 51, 23-31.

Five Other Significant Products

1. **Wang E** (2015). Benchmarking whole-building energy performance with multi-criteria Technique for Order Preference by Similarity to Ideal Solution using a selective objective-weighting approach. Applied Energy, 146: 92-103.

2. **Wang E**, Shen Z, Alp N, Barry N (2015). Benchmarking energy performance of residential buildings using two-stage multifactor data envelopment analysis with degree-day based simple-normalization approach. Energy Conversion and Management, 106: 530-542.
3. **Wang, E.**, Shen, Z., Grosskopf, K. (2014). Benchmarking energy performance of building envelopes through a selective residual-clustering approach using high dimensional dataset. Energy and Buildings, 75, 10-22.
4. **Wang, E.**, Shen, Z., Wang, L., Barry, N. (2014). Benchmarking building energy performance using Data Envelopment Analysis with normalized metrics---A residential case study. Computing in Civil and Building Engineering Conference, ASCE, Orlando, Florida.
5. **Wang, E.**, Shen, Z., Berryman, C. (2011). A building LCA case study using Autodesk Ecotect and BIM model. The 47th ASC Annual International Conference, Omaha, NE.

Synergistic Activities

1. *Professional Activities:*
   - Reviewer for 16 international journals and 15 conference proceedings, e.g., Energy 2015-2016; Energy and Buildings 2016; Journal of Cleaner Production, 2015-2016; Journal of Energy Conversion and Management, 2014-2016; International Journal of Life Cycle Assessment, 2014-2016; Building Simulation 2016; Big Data and Urban Informatics (Springer book) 2015; The 51st ASC Annual International Conference, 2015; LCA XIII conference, 2013
   - Technical committee member of 6 international conferences, e.g., the 11th Conference on Sustainable Development of Energy, Water and Environment Systems (SDEWES), Portugal, 2016; American Center for Life Cycle Assessment-LCAXVI conference, USA, 2016

2. *Major Awards and Registration:* Recipient of the Outstanding Researcher, CECS, 2014-2016; the 2013 Outstanding Graduate Student Award, UNL, 04/18/13; Certified Associate Constructor (AC), 12/20/13; Certified Professional Constructor (CPC), 04/05/14

3. *Related Projects:* Participated in three projects closely related to the proposed research "Advanced decentralized water/energy network design for sustainable infrastructure." USEPA, $1,249,995. 5/09-4/14; "Improving sustainability of atomic layer deposition: a hierarchical systems approach." NSF, $475,752. 07/12-12/14; "Energy Performance of Residential Building Using Simple-Normalization Based Two-Stage Data Envelopment Analysis." THEC-CEACSE, $91,000, 07/15-12/16; "A Systematic Investigation on Principal Energy Determinants of U.S. Residential Buildings", PREP Award, $14,036, 08/01/2016–07/31/2017; "Robust Building Energy Performance Evaluation through Multi-criteria Benchmarking Approach", Ruth S. Holmberg Grant, $3,000, 08/01/2016–12/31/2016; "EXCEL: EXploring Clean Energy through hands-on Learning", NSF, $ 1,192,081(Pending).

4. *Student Training:* Developed two undergraduate-level courses (UTC): Building Information Modeling, Green Building Rating Systems; and two graduate-level courses: Sustainability and LEED, Decision Making and Optimization (UTC) to strengthen sustainability education among undergraduates and graduates.

Jin Wang

Professor and UNUM Chair of Excellence
Department of Mathematics
University of Tennessee at Chattanooga

Professional Preparation

University of Science & Technology of China	Mathematics	B.S.	(1994-1998)
University of Science & Technology of China	Mathematics	M.S.	(1998-2000)
The Ohio State University (Columbus, OH)	Mathematics	Ph.D.	(2000-2004)

Appointments

2014-present	University of Tennessee at Chattanooga	Professor
2012-2014	Old Dominion University	Associate Professor
2007-2012	Old Dominion University	Assistant Professor
2005-2007	Duke University	Assistant Research Professor
2004-2005	The Ohio State University	Lecturer

Products

Related Publications

1. A. Timalsina, G. Hou and **J. Wang**, Computing fluid-structure interaction by the partitioned approach with direct forcing, *Communications in Computational Physics*, vol. 21(1), pp. 182-210, 2017.

2. T. Huynh, G. Hou and **J. Wang**, Communicating wave energy: An active learning experience for students, *American Journal of Engineering Education*, vol. 7, pp. 37-46, 2016.

3. T. Huynh, G. Hou, **J. Wang**, M. Hou and M. Kotinis, A hybrid virtual reality simulation system for wave energy conversion, *International Journal of Computational Engineering Research*, vol. 5(6), pp. 50-60, 2015.

4. G. Hou, **J. Wang** and A. Layton, Numerical methods for fluid-structure interaction - A review, *Communications in Computational Physics*, vol. 12(2), pp. 337-377, 2012.

5. **J. Wang** and G. Baker, A numerical algorithm for viscous incompressible interfacial flows, *Journal of Computational Physics*, vol. 228, pp. 5470-5489, 2009.

Other Publications

1. **J. Wang**, C. Modnak and G. Hou, Convergence analysis of an iterative algorithm for a class of constrained dynamic problems, *Applied Mathematics and Computation*, vol. 219, pp. 1200-1221, 2012.

2. **J. Wang** and A. Layton, New numerical methods for Burgers' equation based on semi-Lagrangian and modified equation approaches, *Applied Numerical Mathematics*, vol. 60, pp. 645-657, 2010.

3. **J. Wang** and A. Layton, Numerical simulations of fiber sedimentation in Navier-Stokes flows, *Communications in Computational Physics*, vol. 5(1), pp. 61-83, 2009.

4. **J. Wang**, An asymptotic expansion for Stokes waves with viscosity, *Fluid Dynamics Research*, vol. 40, pp. 155-161, 2008.

5. **J. Wang**, Computation of 2D Navier-Stokes equations with moving interfaces by using GMRES, *International Journal for Numerical Methods in Fluids*, vol. 54, pp. 333-352, 2007.

Synergistic Activities

- Reviewer: *Journal peer review (more than 50 manuscripts in 30+ journals); Grant panel/review (National Science Foundation, Kentucky Science & Engineering Foundation, Georgian National Science Foundation, etc.); Conference proceedings review (more than 10 conferences); Book review (4 books).*
- Grant activities: *Over 2.2 millions of research and education grants from federal, state and private funding agencies during the last 10 years, including 7 grants from the National Science Foundation.*
- University service: *Curriculum Committee (2009, 2015, 2016), Colloquium Committee (2014, 2015, 2016, 2017), Faculty Search Committee (2009, 2010, 2014, 2015, 2016, 2017), Tenure and Promotion Committee (2015, 2016, 2017), Computational Science Ph.D. Screening Committee (2016, 2017), Internal Research Advisory Group (2016), Doctoral Dissertation Committees (Fernando, 2008; Brown, 2010; Neamprem, 2010; Liao, 2010; Malali, 2012; Modnak, 2013; Posny, 2014; Gounley, 2014; Ghazizadeh, 2014; Malali, 2015; Timalsina, 2017; Edwards, 2017), Qualifying Examination Committees (Li, Posny, Phuworawong, 2011; Malali, 2012; Ghazizadeh, 2013).*
- Honors and awards: *UNUM Chair of Excellence (2014-); Arts & Sciences Dean's Award (2016); NIH Early Career Reviewer Program (2011); Sigma Xi (2009); Faculty Innovator Award (2009); Inclusion in Who's Who in America (2008); Distinguished Graduate Teaching Associate Award (2004).*
- Curriculum development: *Differential equations and dynamical systems (2011); Computational mechanics and fluid-structure interactions (2010); Numerical Linear Algebra (2016); Mathematical Biology (2016).*

Collaborators and Other Affiliations

Advisors

Greg Baker (The Ohio State University, Ph.D. supervisor)
Tom Beale (Duke University, Postdoctoral supervisor)

Collaborators

Antonio Chiocca (The Ohio State University), Fred Dobbs (Old Dominion University), Renee Fister (Murray State University), Avner Friedman (The Ohio State University), Holly Gaff (Old Dominion University), Gene Hou (Old Dominion University), Ravindra Joshi (Old Dominion University), Miltiadis Kotinis (Old Dominion University), Anita Layton (Duke University), Suzanne Lenhart (University of Tennessee), John Glenn Morris (University of Florida), Zindoga Mukandavire (University of Florida), Stephan Olariu (Old Dominion University), Elsa Schaefer (Marymount University), Zhisheng Shuai (University of Central Florida), Jianjun Paul Tian (New Mexico State University), Lucy Zhang (Rensselaer Polytechnic Institute), Xiaopeng Zhao (University of Tennessee)

Graduate advisees

Shu Liao (Ph.D. 2010), Modnak Chairat (Ph.D. 2013), Drew Posny (Ph.D. 2014), Ashlee Edwards (Ph.D. 2017), Asim Timalsina (Ph.D. 2017), Chayu Yang, Dimitri Kakavelakis, Evan Lee, John Gounley, Nathaniel Beckman, Hersh Patel, Ozkan Serttas, Chak Pong Chung, Johnathon Upperman, Kumudu Gamage, ZiQiang Cheng

Undergraduate advisees

Daniel Drake, Alexander Pulman, Brittany Jacques, Mindy Marshall, Ashley Moye, Breanna White, Yong Suk Ko

Appendix B

Awardee Project Reports

New Projects for FY 2018

Dr. Feng Bao, Lead PI

Co-PI(s): Dr. Jin Wang
Project Title: “Computational Modeling and Uncertainty Quantification for Wave Energy”

Date Submitted: 02/27/2017

Award Start - End Date: 07/01/2017-06/30/2018

Non-Technical Summary:
Ocean waves, generated by wind blowing over the water surface, have tremendous energy which can be captured and converted into electricity. With the rising demand for energy, growing consumption of oil and gas, and increasing global warming, waves offer an attractive green energy source and have generated considerable interest in research, development and testing in recent years.

In this project, we focus on the development of computational methods to simulate the complex motion involving ocean waves, wind and energy buoys. Throughout the past year, the team has conducted extensive work on the computation of wind-ocean wave interaction, fluid-structure interaction, RANS simulation and stochastic modeling of the fluid motion. In particular, Dr. Bao studied stochastic modeling and numerical solutions for (stochastic) partial differential equations that can be applied to wave energy modeling and wave energy simulations; Dr. Wang’s work has been focused on the development of deterministic numerical algorithms for computing multi-phase fluid flows and fluid-structure interactions, essential for the investigation of wave energy dynamics. Dr. Feng Bao and Dr. Jin Wang has submitted two research publications throughout the award period and generated several new ideas due to the research supported in this project.

In addition to the research activities conducted in this project, Dr. Feng Bao and Dr. Jin Wang recruited graduate students and incorporated project methods and findings into their research training. Dr. Bao has supervised a M.S. student (Robert Slaughter) who is conducting research in stochastic modeling and computation. Dr. Wang has been mentoring a Ph.D. student (Chayu Yang) and a M.S. student (Conrad Ratchford). Chayu is expected to obtain his Ph.D. in applied/computational math in 2019, and Conrad recently graduated with a M.S. and is entering our applied/computational math Ph.D. concentration in Fall 2018.

Computational Modeling and Uncertainty Quantification for Wave Energy

Technology Area of Interest: Energy and Environment

PROPOSED TECHNICAL APPROACH	OPERATIONAL CAPABILITY PROVIDED
In this project, we develop computational methods to simulate the complex motion of ocean waves, wind, and energy buoys. • Task 1: Construct deterministic computational algorithms for two-phase flows with fluid-structure • interactions • Task 2: Apply RANS solvers to simulate larger scale models • Task 3: Introduce stochastic representations of Navier-Stokes equation to describe uncertainties • in the model and develop corresponding numerical methods	Stochastic modeling and numerical solutions for stochastic partial differential equations that can be applied to wave energy modeling and wave energy simulations have been studied, and numerical algorithms for computing multi-phase fluid flows and fluid-structure interactions have been introduced. In addition to the research activities, solid collaborations have been established between UTC and preeminent national labs, and graduate students are recruited into UTC graduate research programs.
SPECIFIC OUTCOMES	**OTHER INFO**
Publications 1. Z. Cheng, Y. Liu, M. Zhang and J. Wang, IB-WENO method for incompressible flow with elastic boundaries, Journal of Computational and Applied Mathematics, 2018. Acceptance pending on minor revision. 2. F. Bao, L. Mu and J. Wang, A fully computable posteriori error estimate for the Stokes equations on polytopal meshes, SIAM Journal of Numerical Analysis, 2018. Minor revision. **Solid External Collaborations** • Dr. Lin Mu, Oak Ridge National Laboratory • Dr. Zhenyu Huang, Pacific Northwest National Laboratory	**Budget and Schedule** Total Budget: $84,771.00 Actual Used: $67,977.27 Balance: $16,793.73 Total period of performance is 12 months. Task 1: Months 1-4 Task 2: Months 4-8 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work **Organization Information** Department of Mathematics, Dr. Feng Bao EMCS Building, Chattanooga, TN 37403 Telephone: 423-425-4545 Email: feng-bao@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

In this project, we explored the mathematical framework for fluid-structure interface in both the analysis aspect and the computational aspect of the problem. The PI (Dr. Feng Bao) and Co-PI (Dr. Jin Wang) submitted two research articles to major peer review journals and Dr. Jin Wang has presented the work related to the project in two conferences. With the support of this project, the PI invited several researchers from major research institutes to visit UTC. This includes Dr. Zhenyu Huang, IEEE fellow and distinguished research scientist at Pacific Northwestern National Laboratory. Dr. Huang is interested in collaboration with UTC related to

Power Grid problems and would be a potential funding contact from Department of Energy. The PI and Co-PI also established active collaboration with Dr. Lin Mu, a research scientist at Oak Ridge National Laboratory. With Dr. Mu, we are planning a joint proposal to be submitted to National Science Foundation.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Construct deterministic computational algorithms for two-phase flows with fluid-structure interactions	The PI and Co-PI developed computational frame work for two-phase flows with fluid-structure interactions. Two publications are generated based on the research of this task.
Introduce stochastic representations of Navier-Stokes equation to describe uncertainties in the model and develop corresponding numerical methods	The PI introduces a stochastic differential equation which is equivalent to the Navier-Stokes equation. Numerical algorithms are designed and numerical analysis is going on.

Challenges & Strategies Used to Address / Overcome:

The major challenge of the research proposed in this project is to study the boundary between fluid and the structure. We have studied both the boundary condition of the computational system as well as the error analysis related to finite element methods.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

Because the PI left UTC, we didn't complete the stochastic computing part of the project and data assimilation for the model is of our interests, but didn't get change to study this topic. We hope we can continue this part of research in the future.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

With the support of this project, the PI and Co-PI establish solid collaboration with external researchers.

Students Impacted

Three students were recruited to work on this project. Dr. Bao has supervised a M.S. student (Robert Slaughter) who is conducting research in stochastic modeling and computation. Dr. Wang has been mentoring a Ph.D. student (Chayu Yang) and a M.S. student (Conrad Ratchford). Chayu is expected to obtain his Ph.D. in applied/computational math in 2019, and Conrad recently graduated with a M.S. and is entering our applied/computational math Ph.D. concentration in Fall 2018.

Community and Broader Impacts

Presentations:

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

J. Wang, "Computing fluid-structure interaction." Computer Science and Mathematics Division, Oak Ridge National Laboratory, September 2017.

Work products reduced to practice; provide a bibliographical entry where appropriate

Journal publications:

Z. Cheng, Y. Liu, M. Zhang and J. Wang, IB-WENO method for incompressible flow with elastic boundaries, Journal of Computational and Applied Mathematics, 2018. Acceptance pending on minor revision.

F. Bao, L. Mu and J. Wang, A fully computable posteriori error estimate for the Stokes equations on polytopal meshes, 2018. Under review.

New inventions reduced to practice and when they will be formally disclosed;

N/A

Outreach & Collaboration

The PI invited several researchers from major research institutes to visit UTC. This includes Dr. Zhenyu Huang, IEEE fellow and distinguished research scientist at Pacific Northwestern National Laboratory. Dr. Huang is interested in collaboration with UTC related to Power Grid problems and would be a potential funding contact from Department of Energy. The PI and Co-PI also established active collaboration with Dr. Lin Mu, a research scientist at Oak Ridge National Laboratory. With Dr. Mu, we are planning a joint proposal to be submitted to National Science Foundation.

EXTERNAL FUNDING

Proposal Submissions

1. The team has been collaborating with Dr. Lin Mu (ORNL staff and SimCenter adjunct faculty) in the preparation of a joint proposal, partly built on the findings of the current CEACSE project, to the NSF Computational Mathematics program in near future.
2. Meanwhile, Dr. Wang is currently working with his colleague, Dr. Andrew Ledoan, for a math REU proposal that is to be submitted to NSF in August 2018. Some of the methods and results from this CEACES project will be incorporated into the REU proposal.

Contracts/Awards Received

Dr. Bao received the SciDAC project as Co-PI from Department of Energy during his service at UTC. The SciDAC project is short for Scientific Discovery through Advanced Computing. It is a major research effort sponsored by U.S. Department of Energy to encourage collaboration between scientists and computational mathematicians. The research sponsored in the CEACSE project enhanced such collaboration, thus improved the capability for faculty to achieve more prestigious research grants.

Sponsored Program Capacity Building Activities

N/A

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

We will continue our research on stochastic computing on the model we proposed in this project and the data assimilation related to the model.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

We would like to study stochastic optimization problems in light of the support from CEACSE. An important collaboration institute is Pacific Northwest National Laboratory.

Tell us anything else we should know about this work not described above.

N/A

What barriers (if any) do you face to reach these next goals?

N/A

FINANCIAL ACCOUNTING

Total Award Amount: $$84,771.00

Cumulative Expenditures: $67,977.27

Remaining Award Amount: $16,793.73

CEACSE BUDGET Modification

In this project, the major change in the budget is that the budget for summer salary of the PI, Dr. Feng Bao is transferred to the academic salary due to the external coverage for Dr. Bao's salary. Another change is to transfer some of graduate support to undergraduate support. The reason is that we have recruited three undergraduate students to work on the project. Since we didn't spend all the money in the project, we requested to extend the project for another year.

Dr. Bradley Harris, Lead PI, Assistant Professor, Dept. of Civil & Chemical Engineering

Co-PI(s): Dr. David Giles, Assistant Professor, Dept. of Biology, Geology, & Env. Sci.
Other Personnel: Senior Personnel - Dr. Ethan Hereth, HPC Specialist, SimCenter

Project Title: "A computational study of the impact of fatty acid substitutions on Vibrio cholerae outer and inner membranes"

Date Submitted: 02/27/2017

Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
The bacterium *Vibrio cholerae* (*Vc*) is responsible for the acute intestinal infection known as cholera. The ability of this pathogen to scavenge lipids from its environment is a crucial factor in how it is able to adapt and spread disease. Our hypothesis is that one way in which *Vc* utilizes these lipids is for membrane remodeling. To study this, we carried out computational simulations of the *Vc* membranes to analyze the effect of fatty acid substitutions on membrane characteristics. We found that the introduction of exogenous fatty acids causes the outer membrane to become less permeable, while also fixing the portions of the membrane susceptible to antibiotics into a more rigid conformation. These findings support our experimental data on *Vc* membrane permeability and antibiotic resistance in the presence of these fatty acids. Work products from this project include multiple conference presentations, as well as a grant proposal to the National Institutes of Health. A manuscript for submission to a peer-reviewed journal is also currently being drafted. This research has the potential to identify a new class of preventatives and therapeutics for diseases caused by bacterial pathogens. This project supported the mission of the SimCenter by establishing a new multidisciplinary research project in applied computational science on campus, in the priority area of health and biological systems.

A computational study of the impact of fatty acid substitutions on Vibrio cholerae outer and inner membranes

Technology Area of Interest: Energy and Environment

PROPOSED TECHNICAL APPROACH

The overall objective of this research project was to study the effects of fatty acid composition on *Vibrio cholerae (Vc)* membrane characteristics using molecular dynamics simulation.

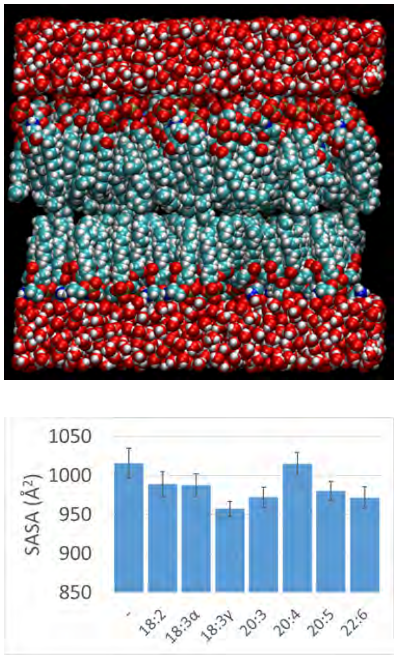
- Task 1: Determine overall structure and approximate composition of *Vc* inner and outer membranes.
- Task 2: Develop models of base case *Vc* inner and outer membranes, as well as modified models of *Vc* inner and outer membranes substituted with exogenous fatty acids of interest.
- Task 3: Conduct molecular dynamics simulations of the membrane models and analyze simulation results to determine effect of fatty acid substitutions on membrane characteristics.
- Task 4: Present findings at regional/national conferences, include as preliminary data in external grant proposals, and prepare draft manuscript.

SCIENTIFIC DISCOVERY PROVIDED

This computational study has led to the discovery of molecular-level phenomenon that take place in bacterial membranes as a result of environment-induced membrane remodeling. This research project is part of a larger study of the ability of bacteria to uptake environmental lipids and the implications for persistence and pathogenicity. Bacterial pathogens are increasingly developing resistance to conventional antibiotics, which typically target in vitro viability. One potential solution is to target the fatty acid uptake and utilization pathways, which regulate functions that are critical to the ability of these pathogens to persist and spread disease. Thus, this research could lead to the development of a novel class of preventatives and therapeutics for bacterial diseases.

RESULTS

Figure 1. Side view (top) and solvent-accessible surface area (bottom) of the *Vibrio cholerae* outer membrane.



OTHER INFO

Budget and Schedule

Total Budget:	$27,481.00
Actual Used:	$27,415.50
Balance:	$ 65.50

Total period of performance is 12 months.

Task 1: Months 1-2
Task 2: Months 3-6
Task 3: Months 5-12
Task 3: Months 9-12

Deliverables

- Monthly report describing numerical methods, techniques, and results that were developed or improved.
- Final report detailing results, financials, and future work

Organization Information

UTC CECS, Dr. Bradley Harris
615 McCallie Avenue,
Chattanooga, TN 37403
Telephone: 423-425-2209
Email: Bradley-Harris@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The central hypothesis of this research is that the bacterial pathogen *Vibrio cholerae* (*Vc*) utilizes exogenous fatty acids for membrane remodeling, in order to adapt to its environment and spread disease. We have collected experimental data that supports this hypothesis, but lack a molecular-level understanding of how assimilation of these fatty acids contributes to experimentally observed membrane adaptation. Thus, the overall objective of this research project was to study the effects of fatty acid composition on *Vc* membrane characteristics using molecular dynamics simulation. This was accomplished via the pursuit of two specific aims to identify the extent to which exogenous fatty acid assimilation: (1) contributes to changes in membrane permeability; and (2) alters membrane susceptibility to antibiotics. Membrane models were built using in-house scripts written in VMD, and molecular dynamics simulations were carried out using NAMD with the modified CHARMM force field on a SimCenter cluster. Membrane permeability and susceptibility to antibiotics were quantified via solvent-accessible surface area and the membrane order parameter, respectively. This data was calculated from simulation trajectory data using in-house scripts written in VMD. We found that assimilation of exogenous fatty acids results in decreased solvent-accessible surface area, which means that the membrane becomes less permeable. We also found that fatty acid substitutions result in increased order in those portions of the membrane susceptible to antibiotics. This means that the membrane becomes more rigid, which could impact its resistance to antibiotics. These computational results support our experimental data on *Vc* membrane permeability and antibiotic resistance in the presence of exogenous fatty acids.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop models of base case *Vc* inner and outer membranes	• Base case inner membrane was constructed as a symmetrical bilayer of 128 molecules of dipalmitoyl phosphatidylethanolamine (PE) and phosphatidylglycerol (PG). A composition of 75% PE and 25% PG was assumed based on available literature. • Base case outer membrane was constructed as an asymmetrical bilayer, consisting of an outer leaflet of 32 lipid A molecules, and an inner leaflet of 64 PE and PG molecules. The composition of the inner leaflet was again assumed to be 75% PE and 25% PG.
Develop modified models of *Vc* inner and outer membranes substituted with exogenous fatty acids of interest	• Modified models of the inner membrane were constructed by randomly substituting 50% of the sn2 chains with a specific fatty acid of interest. Modified models were developed for each of the following fatty acids: 18:2, 18:3α, 18:3γ, 20:3, 20:4, 20:5, 22:6. • Modified models of the outer membrane were constructed by randomly substituting 50% of the sn2 chains in the inner leaflet with a specific fatty acid of interest.

	Modified models were developed for each of the following fatty acids: 18:2, 18:3α, 18:3γ, 20:3, 20:4, 20:5, 22:6.
Conduct molecular dynamics simulations of the membrane models	• Each membrane model was solvated with water molecules, subjected to 50 ps of energy-minimization, and then equilibrated for at least 1 ns. Molecular dynamics (MD) production runs were then carried out for 5 ns.
Analyze simulation results to determine effect of fatty acid substitutions on membrane characteristics	• Simulation trajectory data was analyzed to determine the effect of fatty acid substitutions on the following membrane characteristics: solvent accessible surface area, and lipid tail order parameter.
Present findings at regional and national conferences	• Research findings were presented at the 2018 UTC RESEARCH Dialogues, as well as the 2018 American Institute of Chemical Engineers (AIChE) Southern Regional Conference.
Publish findings in a peer-reviewed journal	• A manuscript is currently being drafted, with an anticipated submission date of Summer 2019.
Include findings as preliminary data in external grant proposals	• Dr. Harris submitted a grant proposal as PI in February 2018 to the National Institutes of Health Small Grant Program (NIH R03) related to this project.

Challenges & Strategies Used to Address / Overcome:

The performance of NAMD on the SimCenter cluster was not as efficient as anticipated. This was not a problem for the membrane simulations because of the relatively small number of atoms, but this will need to be addressed for future studies (particularly those involving membrane-embedded proteins).

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

All research goals were met. However, graduate student support will be critical for the success of follow-up research related to this project. Dr. Harris carried out the simulations and subsequent analyses for this project on his own, but this will not be practical for subsequent research.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

Harris (PI): The work products resulting from this research project, particularly the NIH R03 grant proposal and the anticipated manuscript submission, bolster the PI's research portfolio for pursuit of tenure and promotion. Furthermore, these work products enhance the PI's reputation in this field, increasing the likelihood of funding for future external grants, as well as the potential for future partnerships with other researchers. For example, Dr. Harris has been added as a faculty research mentor for an NSF REU resubmission by Dr. Hong Qin (see below for details).

Giles (Co-PI): With a research portfolio bolstered by this and other interdisciplinary research projects, Dr. Giles applied for and received promotion and tenure in Spring/Summer 2018.

Students Impacted

None.

Community and Broader Impacts

- Technical impacts: This computational study has led to the discovery of molecular-level phenomenon that take place in bacterial membranes as a result of environment-induced membrane remodeling. These findings will be used as preliminary data for future external grant proposals to extend the scope of this research study. Potential avenues for future computational research include simulating bacterial membranes in the presence of antibiotics or antimicrobials, as well as studies of relevant membrane-embedded proteins. These efforts will be coupled with experimental research aimed at evaluating changes in bacterial phenotypes in the presence of exogenous fatty acids over a range of environmental conditions.
- Institutional impacts: Future external grants enabled by this award will be used to recruit undergraduate and graduate researchers, which will serve to enhance student learning and development through involvement in cutting-edge research. This work will also serve to strengthen our research expertise through enhanced applied research capabilities and improved national/international recognition. Lastly, this project has the potential to result in future collaborations with external government organizations with whom the PI has previously collaborated (e.g. ORNL), as well as local community partners (e.g. Erlanger Children's Hospital).
- Societal impacts: This research project is part of a larger study of the ability of bacteria to uptake environmental lipids and the implications for persistence and pathogenicity. Bacterial pathogens are increasingly developing resistance to conventional antibiotics, which typically target in vitro viability. One potential solution is to target the fatty acid uptake and utilization pathways, which regulate functions that are critical to the ability of these pathogens to persist and spread disease. Thus, this research could lead to the development of a novel class of preventatives and therapeutics for bacterial diseases.

Work products reduced to practice; provide a bibliographical entry where appropriate

Presentations:

Boeger, Doyle, Giles, Harris. Studying environmental persistence and virulence factors of Vibrio cholerae in marine and human host environmental conditions. Poster presented at: American Institute of Chemical Engineers Southern Regional Conference; 2018 April 7; Baton Rouge, LA (Non-refereed Conference).

Doyle, Boeger, Giles, Harris. Influence of environmental conditions on fatty acid-induced changes in Vibrio cholerae persistence and pathogenicity. Poster presented at: Southern Regional Honors Conference; 2018 April 7; Arlington, VA (Non-refereed Conference).

Harris. Exploring the impact of the marine-to-host environmental transition on persistence and pathogenicity in Vibrio cholerae using a DOE approach. Presentation given at: UTC RESEARCH Dialogues; 2018 April 3; Chattanooga, TN (Non-refereed Conference).

Turgeson, Boeger, Giles, Harris. Introducing biochemistry and cellular biology to chemical engineering students by cultivating a bacterial pathogen in a bioreactor. Paper presented at: American Society for Engineering Education Southeastern Section Conference; 2018 March 5; Daytona, FL (Refereed Conference).

New inventions reduced to practice and when they will be formally disclosed

None.

Outreach & Collaboration

None.

EXTERNAL FUNDING

Proposal Submissions

1. NIH Small Grant Program (R03); PI: Harris; Title: The impact of the marine-to-host transition on fatty acid-induced changes in persistence and pathogenicity in Vibrio cholerae; Budget: $100k, Duration: 2 yrs; Submitted: February 2018
2. NIH AREA (R15); PI: Wang; Senior Personnel: Giles, Harris; Title: Experimentally guided modeling and simulation for cholera dynamics; Budget: $250k, Duration: 3 yrs; Submitted: February 2018
3. CEACSE Award; PI: Wang, Co-PIs: Giles, Harris; Title: Waterborne infections and pathogen dynamics: modeling, experimentation, and large-scale computation; Budget: $100k, Duration: 1 yr; Submitted: March 2018

Contracts/Awards Received

1. CEACSE Award; PI: Wang, Co-PIs: Giles, Harris; Title: Waterborne infections and pathogen dynamics: modeling, experimentation, and large-scale computation; Award Amount: $100k, Duration: 7/1/18-6/30/19; Sponsor: UTC SimCenter
2. Faculty Pre-Tenure Enhancement Award; PI: Harris, Title: Studying the physiological and behavioral adaptations of pathogenic bacteria in an effort to improve disease control strategies; Award Amount: $15k, Duration: 7/1/17-6/30/18; Sponsor: UTC Office of Research and Sponsored Programs
3. Ruth S. Holmberg Grant for Faculty Excellence; PI: Harris; Title: Studying bacterial physiological and behavioral adaptations in an effort to improve disease treatment and prevention strategies; Award Amount: $5k, Duration: 7/1/17-6/30/18; Sponsor: UTC Provost's Office

Sponsored Program Capacity Building Activities

Dr. Harris (PI): Participated in a GWSW grant-writing cohort sponsored by the UTC CECS in Summer 2017; attended the NIH Regional Seminar on Program Funding and Grants Administration in May 2018; attended two on-campus viewing sessions of NSF CAREER webinars in May 2018.

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

In the short-term, these simulations will be repeated at different environmental conditions (e.g., temperature, pH, salinity) to determine how the environment influences fatty acid-induced changes in membrane characteristics. Antibiotics (e.g., polymixin B) and antimicrobials (e.g., LL-37, HBD-1, HBD-2) will also be introduced to the simulations to determine the molecular mechanisms by which these molecules destabilize bacterial membranes and examine what effect, if any, fatty acid modifications have on these processes. Long-term, this simulation study will be extended to include membrane-embedded proteins of interest. These include the outer membrane transporter protein FadL, as well as the fatty acyl coenzyme A ligase FadD.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

During the course of presenting research findings from the CEACSE award, Dr. Harris was introduced to Dr. Hong Qin, Associate Professor in Computer Science and Engineering at UTC. Dr. Harris will be participating in Dr. Qin's upcoming NSF REU resubmission as senior personnel (faculty research mentor). He will be offering a research project to site participants that follows up on the CEACSE award research. In light of Dr. Qin's broad expertise in systems

biology and gene network modeling, Dr. Harris envisions future collaborations in other research areas as well, such as biofuels production and renewable routes to commodity chemicals.

Dr. Giles, because of his continued involvement in this project, has established a collaboration with Myriam Cotten, an associate professor at the College of William and Mary. Dr. Cotten studies the mechanisms of fish antimicrobial peptides on bacterial membranes. She has offered to send peptides for testing of MIC using V. cholerae, which is likely to lead to membrane modeling studies to examine the peptide-membrane interactions.

What barriers (if any) do you face to reach these next goals?

Support for graduate and undergraduate student researchers will be critical for future success.

FINANCIAL ACCOUNTING

Total Award Amount: $27,481.00

Cumulative Expenditures: $27,415.50

Remaining Award Amount: $65.50

Category	Amount Requested	Funds Spent
A. Senior Personnel		
1. PI: Dr. Bradley J. Harris		
Dr. Harris will work 1 summer month on this project. His 9-month salary is $83,636; for 1 month is $9,293 x 3% raise = $9,572	$9,572	$1,867
75 hours extra service pay Aug.-Dec. 2017 (15 hr/month for 5 months @ $64.71/hr)		$4,853
58 hours extra service pay Jan.-April 2018 (15 hr/month for 4 months @ $64.71/hr)		$3,753
8 hours summer pay May 2018 @ $64.71/hr		$518
2. Co-PIs		
Co-PI: Dr. David Giles		
Dr. Giles will work 0.5 summer months on this project. His 9-month salary is $60,649; for 1 month is $6,739 x 3% raise = $6,941 x 0.5 months = $3,470	$3,470	$901
40 hours extra service pay Aug.-Dec. 2017 (8 hr/month for 5 months @ $44.83/hr)		$1,793
32 hours extra service pay Jan.-April 2018 (8 hr/month for 5 months @ $44.83/hr)		$1,435
4 hours summer pay May 2018 @ $44.83/hr		$179
Co-PI: Dr. Ethan Hereth		
Dr. Hereth will work 14 days on this project; calculation is based on 224 duty days per academic year. His 12-month salary is $85,600/224 is $382 x 3% raise = $394 x 14 days = $5,511	$5,511	$5,511
B. Fringe Benefits		
PI: Dr. Bradley J. Harris (35% of salary)	$3,350	$1,810
Co-PI: Dr. David Giles (54% of salary)	$1,874	$1,153
Co-PI: Dr. Ethan Hereth (40% of salary)	$2,204	$2,143
D. Travel		
a. Domestic		

Travel to the American Chemical Society National Meeting being held in New Orleans, LA from March 18th-22nd, 2018.	$1,500	
Travel to the AIChE 2018 Southern Regional Conference for Dr. Harris and an undergraduate student in April 2018		$1,500
TOTAL FUNDS REQUESTED/SPENT	$27,481	$27,416

Dr. Harris was the PI of this project and the researcher responsible for developing the membrane models, conducting the molecular dynamics simulations, and analyzing the resulting trajectory data. He is also the primary writer and corresponding author on resulting presentations and publications. We originally budgeted one month of summer salary for him to conduct this research. Due to time constraints and other obligations during the summer, this research continued into the academic year. Dr. Harris received summer pay and extra service pay accordingly (see Table 1 above).

Dr. Giles was the biology expert and experimental collaborator on this project. He was responsible for assisting in membrane model development, which was based on his experimental data. He also assisted in reviewing simulation data for biologically relevant results and conclusions, and is an author on resulting presentations and publications. We originally budgeted a half-month's summer salary for his work on this project. Due to time constraints and other obligations during the summer, this research continued into the academic year. Dr. Giles received summer pay and extra service pay accordingly (see Table 1 above).

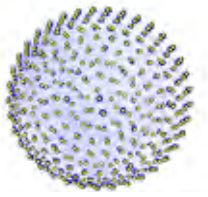
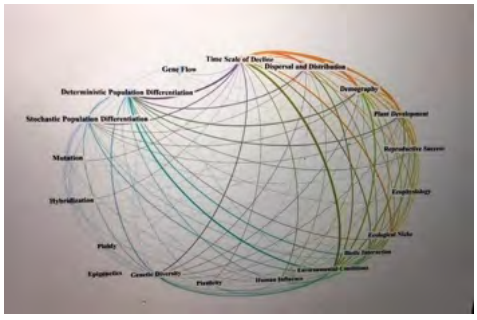
Dr. Hereth was the scientific computing expert and the primary contact at the SimCenter. He was responsible for the setup and installation of NAMD on the current computing architecture available at the SimCenter, and provided assistance in troubleshooting any issues with running NAMD on these computing resources. We originally requested two week's salary for Dr. Hereth, and he was paid as such.

We originally budgeted for airfare, lodging, and conference registration for Dr. Harris to present this work at the ACS National Meeting in New Orleans, LA in March 2018. Instead, this work was presented by an undergraduate student at the AIChE 2018 Southern Regional Conference in Baton Rouge, LA in April 2018.

Dr. Hope Klug, Lead PI

The Development and Application of Computational Tools to Address Fundamental Questions in Ecology and Evolution

Technology Area of Interest: Health and Biological Systems

PROPOSED TECHNICAL APPROACH	FINDINGS
The primary goal of the research is to develop and utilize computational tools for addressing ecological and evolutionary questions using big datasets. • Task 1: Develop tools to utilize big data sets in biology • Task 2: Apply these tools to examine if biological traits are linked to species rarity. • Task 3: Apply these tools to explore how life history, ecology, and sociality interact to influence mating and parental care. • Task 4: Prepare results for publication and apply for additional funding.	Computational network analysis can be used to allow researchers to utilize big data to address questions in ecology and evolution. Our results suggest that 1) there are strong links between ecology, life history, mating strategies, and parental investment and 2) biological traits are linked to species' rarity and that rarity influences climate change vulnerability.
RESULTS	**OTHER INFO**
Figure 1: Links between ecology, life history, mating and parental investment (top image) and links between species' rarity and ecological factors of interest (bottom image)  	**Budget and Schedule** Total Budget: $88,998.00 Actual Used: $88,998.00 Balance: $ 0.00 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-12 Task 3: Months 3-12 Task 3: Months 4-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work **Organization Information** UTC, Dr. Hope Klug 615 McCallie Avenue, Chattanooga, TN 37403 Telephone: 423-425-4225 Email: Hope-Klug @utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview
The project allowed us to:

1. Develop and refine computational tools to address pressing questions in biology; specifically, we have developed the resources to allow us to use computational network analysis to examine links between ecology, evolution, physiology, and abiotic factors.
2. Examine the hypothesis that biological traits are linked to species' rarity and that rarity influences climate change vulnerability; our network analysis research on this topic thus far has allowed us to begin to identify the factors that are most likely linked to and studied in research related to species' rarity.
3. Examine the hypothesis that life-history traits, ecological conditions, and sociality interact to influence mating and parental dynamics; our network analysis research on this topic suggests strong links between ecology, life history, mating strategies, and parental investment.
4. Train numerous graduate and undergraduate students in computational biology; our CEACSE funding allowed us to train seven undergraduate students and two graduate students in network analysis. Given that Biology students at UTC have previously received little to no training in computational biology, this student training has been invaluable. Several of the undergraduate students now plan to attend graduate school, and one of the graduate students is now planning to pursue his Ph.D. in Computational Science at UTC.
5. Submit new grant proposals; the CEACSE-related research facilitated the submission of several new grants, one of which has been recommended for funding with Dr. Qin as the lead PI.
6. Prepare high-impact publications; publications focused on species' rarity and life history evolution are in preparation for submission.
7. Present our research at a national conference; in August, our students will present the research focused on species' rarity at the Ecological Society of America conference.
8. Present our research regionally; two CEACSE-related posters were presented at UTC's Research Dialogues in 2018.

In summary, our CEACSE research has expanded: 1) the tools that biologists can use to address pressing questions in evolution and ecology; 2) our understanding of why some species are rare whereas others are common; and 3) our understanding of the link between ecology, evolution, and social behaviors.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
1. Develop tools to utilize big data sets in biology	During Summer 1 and Semester 1 of our project, Dr. Qin provided substantial training to graduate student Zachary McCoy in the development and refinement of computational tools to address broad biological questions. Dr. Qin and Zachary McCoy then identified ways in which computational network analysis and big data can be used in studies of ecology and evolution. During Summer 1 and Semester

	1, Drs. Klug and Boyd familiarized themselves with computational network analysis and the potential for its use in biology.
2. Apply these tools to examine if biological traits are linked to species rarity.	During Semester 2 and Summer 2 of our project, Dr. Boyd and her research team used computational network analysis to address questions related to species' rarity.
3. Apply these tools to explore how life history, ecology, and sociality interact to influence mating and parental care.	During Semester 2 and Summer 2 of our project, Dr. Klug and her research team used computational network analysis to address questions related to ecology, evolution, and sociality.
4. Publish findings.	At least two manuscripts are in preparation. We expect that at least one of these manuscripts will be submitted in 2018, and the other manuscript is likely to be submitted in 2019. Additional manuscripts are anticipated to result from our CEACSE-funded research.
5. Apply for external funding.	A Letter of Intent was submitted for the National Science Foundation's (NSF) Rules of Life Program, although a full proposal was not invited. An NSF REU proposal (REU Site: ICompBio - Engaging Undergraduates in Interdisciplinary Computing for Biological Research) was submitted but not funded. An NSF BD Spoke proposal was submitted and funded, with Dr. Qin as the lead PI.
6. Train UTC students throughout the grant period.	Our CEACSE funding allowed us to train seven undergraduate students and two graduate students in network analysis. Students have been engaged in all aspects of the research.

Challenges & Strategies Used to Address / Overcome:

No major challenges were encountered that prevented us from achieving our goals. Minor challenges were as follows: 1) given the inter-disciplinary nature of the research, substantial time was required for all three PIs and the students to gain the skills necessary to use relevant computational tools; 2) different databases use varying terms to refer to a single variable (e.g. some databases will use lifespan, whereas others will use longevity), and this required standardization, which has taken additional time; 3) the funding climate in biology is challenging, which means that multiple proposals must be submitted. These were in general expected challenges, though.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

Most aspects of our research worked. However, in general, this project allowed the biology PIs to become aware of challenges (and strengths) associated with the use of computational tools and big data in biology.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

The impact on the careers of the PI and Co-PIs has been transformative. Drs. Boyd and Klug were previously not using big data to address biological questions. This project has provided these researchers with the tools to use big data in their research, which has significantly enhanced their funding and collaborative opportunities and potential. The project additionally facilitated collaboration among three researchers who have not previously collaborated and who, prior to this grant, had no intent to collaborate.

Students Impacted

Braley Gentry, B.S. in Biology underway: student co-led network analysis research related to species rarity. This student is expected to be a co-author on at least one publication and is a co-author on two presentations.

Destinee Jones, B.S. in Biology 2018: student assisted with data extraction and organization related to evolutionary ecology research. This student has been accepted to a graduate program.

Zachary McCoy, M.S. in Environmental Science underway with plans to complete his PhD in Computational Science: this student conducted research related to the use of network analysis in evolutionary biology. This student will likely be the first student from our department to pursue a PhD in Computational Science. He is expected to be the lead author on at least one CEACSE-related publication and he is a co-author on two presentations related to this project.

Madelyn Momchilov, B.S. in Biology 2018: this student assisted with life-history, mating, and parental investment data extraction and organization.

Zachary Sheckley, B.S. in Biology 2018: this student assisted with data extraction and organization related to evolutionary ecology research. This student is expected to be a co-author on at least one publication.

Kaitlyn Smith, B.S. in Biology underway: this student assisted with data extraction and organization related to species rarity research.

Kaitlin Sons, B.S. in Biology underway: this student assisted with data extraction and organization related to species rarity research.

Thomas Wiegand, B.S. in Biology underway: this student co-led network analysis research related to species rarity. This student is expected to be a co-author on at least one publication and is a co-author on two presentations.

Community and Broader Impacts

The research enhanced our understanding of ecology and evolution at a broad scale and provided novel computational tools for utilizing big data in biology. Several students received hands-on training in computational biology research. Additionally, graduate student Zachary McCoy is a teacher at Chattanooga's STEM School and has been presenting his research activities to his high school students.

Work products reduced to practice; provide a bibliographical entry where appropriate

Non-refereed conference:

Hope Klug, Zachary McCoy, Jennifer Boyd, and Hong Qin. Using big data to address fundamental questions in ecology and evolution. Poster Presentation, UTC Research Dialogues, April 2018.

Thomas Wiegand, Braley Gentry, Zachary McCoy, Jared Odell, Hope Klug, Jennifer Boyd. Network Analysis as a method of visualizing connectivity in ecological concepts. Poster Presentation, UTC Research Dialogues, April 2018.

Refereed conference:

Braley Gentry, Thomas Wiegand, Zachary McCoy, Jared Odell, Hope Klug, Jennifer Boyd. Visualizing connectivity of ecological and evolutionary concepts – an exploration of research on species rarity. Poster Presentation, Ecological Society of America Conference. To be presented in August 2018.

Publications are in preparation for submission, but no publications have yet resulted from this project.

New inventions reduced to practice and when they will be formally disclosed

None.

Outreach & Collaboration

Graduate Student Zachary McCoy travelled to the University of Oxford to initiate computational biology collaborations with Professor Mike Bonsall. During this trip, Zachary was able to network and meet with a variety of researchers who use big data in biology at Oxford.

EXTERNAL FUNDING

Proposal Submissions

1. A Letter of Intent was submitted for the National Science Foundation's (NSF) Rules of Life Program, although a full proposal was not invited.
2. An NSF REU proposal (REU Site: ICompBio - Engaging Undergraduates in Interdisciplinary Computing for Biological Research) was submitted but not funded.
3. An NSF BD Spoke proposal was submitted and funded, with Dr. Qin as the lead PI.

Contracts/Awards Received

1. Dr. Qin's NSF BD Spoke proposal, "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education," was funded for $549,888.

Sponsored Program Capacity Building Activities

Dr. Qin's NSF BD Spoke proposal, "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education," was funded for $549,888.

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

In the next year, we will finalize the research products associated with this project. In particular, we expect to have multiple publications associated with this work submitted during the next twelve months. In the next 1-5 years, we will expand upon the foundation that now exists for our computational biology research programs. Dr. Qin, who has extensive experience with network analysis, will continue using computational approaches to address broad biological questions. Drs. Boyd and Klug now have the tools to incorporate network analysis into their own research programs. Dr. Boyd will continue to expand the use of computational tools in her research program focused on species' rarity, and Dr. Klug will now utilize big data in her research program focused on evolutionary ecology. Over the next year, we will also collaboratively use computational tools to better understand the fundamental rules that govern life. Over the next 1-5 years, we anticipate multiple grant submissions, publications, and presentations. We

additionally all plan to expand our interactions with the SimCenter and our supervision of undergraduate and graduate students in computational biology.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

This initial CEACSE-funded research sparked a collaboration between Drs. Klug, Boyd, and Qin, three scientists who had previously not collaborated. We will continue our collaborative efforts in the future, and we will include Dr. Azad Hossain, an expert in geospatial science, in our future work that will be focused on better understanding the fundamental rules that govern life.

Tell us anything else we should know about this work not described above.

This CEACSE project was productive and transformative; it allowed three researchers to expand their approaches to addressing biological questions, it facilitated new collaborations, and it allowed for multiple students to be trained in computational biology. Drs. Boyd and Klug, in particular, had no plans to use network analysis in their research prior to this project.

What barriers (if any) do you face to reach these next goals?

In the future, it will be critical for UTC to provide substantial support to research intensive faculty. Substantial course releases for faculty who secure big grants, for instance, are important to allow faculty to conduct high-impact research. Modernized requirements for graduate theses and dissertations would also be beneficial; for example, allowing students to format theses and dissertations in a manner that is consistent with journals in their field (as is done at a range of research-intensive national and international universities) would greatly facilitate the likelihood that chapters will be quickly submitted for publication.

FINANCIAL ACCOUNTING

Total Award Amount: $88,998.00

Cumulative Expenditures: $88,998.00

Remaining Award Amount: $0.00

Dr. Soubantika Palchoudhury, Lead PI

Co-PI(s): Dr. Abdollah (Abi) Arabshahi
Other Personnel:
Graduate Students (M.S. Chemical Engineering): Uday Gharge, Abdulaziz Albattah

Undergraduate students (Chemical Engineering)*:* Justin Miller, Ketan Patel, Olivia George, Erin Conway, Cody Flowers

Project Title: "Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs"

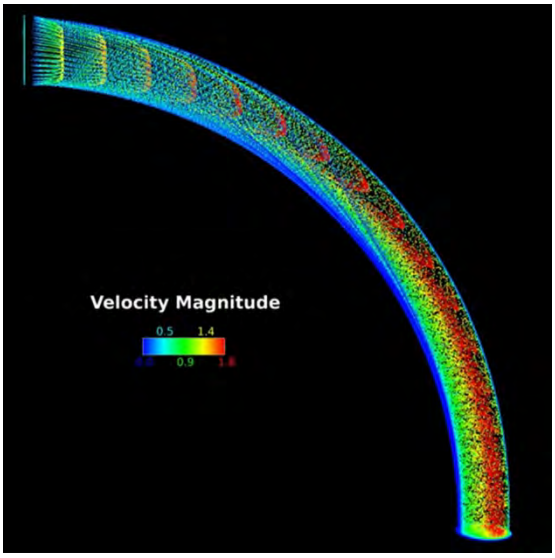
Date Submitted: 02/27/2017

Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
Nanodrugs (*e.g.,* Doxil) are seen as next-generation solution in the field of biomedicine, particularly for their use as chemotherapeutic and drug delivery agents. The key advantage of nanodrugs (at least one dimension < 100 nm) is their ability to selectively reach the diseased site without affecting the healthy tissues. Therefore, a fundamental question in nanomedicine is how to accurately predict the transport and bio-distribution of the new nanodrug within the body. This is near-impossible to determine from a solely experimental viewpoint. In nanomedicine, a computational approach is used to predict the transport and distribution profile of nanodrugs inside the body, but the method is still in its developmental stages. The goal of this project is to develop a computational model in-house at UTC for predicting the transport of a new Pt-iron oxide nanodrug synthesized at CECS (UTC). Transport of nanodrugs is a complex process due to the combined involvement of hydrodynamic forces, chemical interaction of the surface, magnetic attraction, adhesion to the cell wall, and Brownian forces. This project developed a robust and preliminary computational fluid dynamics model to predict this transport and to determine the factors dominating the drug's transport. First, physiological geometries for the path of the nanodrug inside the body was generated from literature. The next step was to develop the mesh or grid through available software. Finally, the flow of the nanodrug was analyzed using *Tenasi*, a flow-solver developed at UTC. Such a model will have immense significance in the biomedical field for designing new and efficient chemotherapeutic nanodrugs. This research directly aligns with the SimCenter's focus area and mission in Health and Biological Systems. The project will put SimCenter at the forefront of emerging innovation in the field of Health and Biological Systems. In addition, the project has tremendous potential for publication in high-impact journals due to its novelty. This research has resulted in one article in the reputed journal of RSC Advances. Another article is currently in submission in the Journal of Magnetism and Magnetic Materials. The project also served to provide preliminary data for extramural funding opportunities in NSF and NIH to be pursued collaboratively by the P.I. and co-P.I.

Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs

Technology Area of Interest: Health and Biological Systems

PROPOSED TECHNICAL APPROACH	FINDINGS
The primary goal of this research is to develop a CFD model and corresponding experimental method to determine transport of nanodrugs • The primary goal of this research is to develop a CFD model and corresponding experimental method to determine transport of nanodrugs • Task 1: Synthesis of a new nanodrug and experimental flow study • Task 2: Build meshes for the flow path • Task 3: Carry out simulation for velocity and mass loss of the nanodrug using the meshes built in Task 2 and experimental Reynolds number of the nanodrug • Task 4: Compare the computational and experimental results, submit papers to peer-reviewed journals, and external proposal preparation.	The computational fluid dynamic (CFD) model developed will provide the capability to predict flow velocity and binding affinity of new nanoscale therapeutics through channels. The experimental approach will be able to complement and validate our computational findings.
RESULTS	**OTHER INFO**
Fig 1: Velocity of nanodrug through 89° bent channel using CFD 	**Budget and Schedule** Total Budget: $99,221.00 Actual Used: $98,665.46 Balance: $ 555.45 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-6 Task 3: Months 6-12 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication • External and internal conference presentation **Organization Information** UTC -Civil and Chemical Engineering Dr. Soubantika Palchoudhury (PI) 615 McCallie Ave, EMCS 440B Chattanooga, TN 37403 Telephone: 423-425-5455 Email: Soubantika-Palchoudhury@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

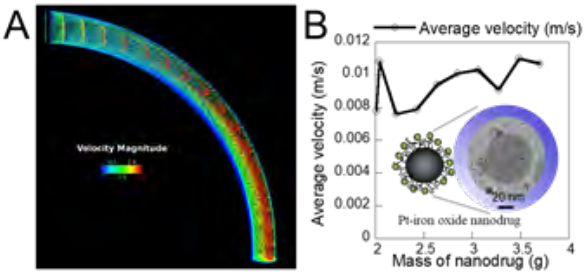


Figure 1. Velocity profile of nanodrug through 89° bent channel. (A) CFD model results and (B) experimental velocity; inset show the Pt-iron-oxide nanodrug.

Nanotechnology is seen as a next-generation tool for biomedical applications like drug delivery. For example, liposome encapsulated doxorubicine or Doxil, one of the first antitumor nanodrug approved by the Food and Drug Administration showed superior bio-distribution and clinical function as compared to free doxorubicine. Accurately predicting transport and accumulation of the nanodrug in the body is a major step for its practical applicability. This is a near-impossible task from a solely experimental approach because several factors like the size, shape, and local flow conditions of the specific nanodrug are likely to play influencing roles. ***The goal of this project was to develop a computational model in-house at UTC for predicting the transport profile of a new chemotherapeutic nanodrug synthesized at CECS***, composed of hybrid Pt-iron oxide nanoparticles (NPs). Using Pt-iron oxide NPs as our experimental system, this project established a robust computational fluid dynamics (CFD) protocol to analyze their transport for two possible drug delivery routes, through straight and 89-degree bent channels. Specifically, the velocity and binding affinity of the nanodrug was assessed via in silico and experimental methods. The results from both techniques were in close agreement. Figure 1 shows the velocity profile of the new nanodrug. This computational solution will be the key in designing suitable next-step in-vivo experiments to determine the efficiency of the drug.

The project has resulted in one journal publication, one journal publication in submission, five conference presentations, collaborations with Sandia National Laboratory, and two potentially patentable products.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Selecting talented undergraduate and graduate students to work on the project and supporting them through the grant	Synthesis of a new Pt-iron oxide nanodrug
Establishing collaboration with CINT, Sandia National Lab for material characterization (electron microscopy and small-angle x-ray scattering) for the project.	Development of a new computational fluid dynamics approach to predict velocity and binding of the new nanodrug through different geometries
Synthesizing Pt-iron oxide nanodrug samples for use in transport experiments Characterizing size and morphology of nanodrugs using CINT facilities	A novel experimental technique to analyze the flow of nanodrugs and compare it with computational results
Extensive literature review on a) major factors impacting the transport of nanodrugs, b) models used for nanoparticle transport, and c) experimental designs Setting up a new and facile experimental method to measure parameters related to nanoparticle transport, based on extensive search for laboratory supplies and equipment from Fisher Scientific, Sigma Aldrich, Bruker, and Malvern Scientific websites	One publication in the journal of RSC Advances (impact factor 2.936) One publication in submission in the Journal of Magnetism and Magnetic Materials (impact factor 3.046) Internal and external conference presentations
Using computational fluid dynamic tools to predict, understand, and validate the flow of these nanodrugs	Tuition support, monthly assistantship, and research training opportunity for graduate students Support and research training for undergraduate students
Conference presentation by the students Publication	Collaboration with Sandia National Lab

Challenges & Strategies Used to Address / Overcome:

Due to the novelty of the project, challenges were encountered in finding relevant literature. The P.I. and co-P.I. resolved this issue through collaborative scientific discussions and combining methods from different fields to sequentially solve the scientific question.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

N/A

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

The grant has been used to start-up and build the P.I.'s Integrated Nanobiomaterials Laboratory at UTC. The laboratory station is currently equipped with state-of-the-art equipment for nanomaterial synthesis and characterization including a fully-functional Schlenk line set-up, ultraviolet-visible (UV-vis) and fourier transform infra-red (FT-IR) spectroscopes, spin coater, Litesizer Particle Analyzer, NanoDrop fluorescence spectroscope, Ultra-pure water purifier, and E-gel electrophoresis system. This project has been a key towards establishing the P.I.'s research collaborations, lab start-up, student support, and publications. The P.I. and co-P.I. are currently pursuing NSF and NIH grants based on the findings from this project.

Students Impacted

Two graduate students and five undergraduate student researchers were trained in the emerging field of development of nanoparticle drugs for next-generation medicine through this project. Details are as follows:

- Uday Gharge, M.S. Chemical Engineering, Thesis, graduated May 2018
- Abdulaziz Albattah, M.S. Chemical Engineering graduate student, Project, graduation in Aug 2018
- Justin Miller, undergraduate student (Chemical Engineering), graduated May 2018; this project helped him gain experience in wet chemical synthesis, material characterization, conference presentations, journal publication, and led to his job at WR Grace Chattanooga
- Ketan Patel, undergraduate student (Chemical Engineering), graduation in Dec 2018; the project helped him gain expertise in nanomaterial synthesis, agricultural application of nanoparticles, conference presentation, and journal publication
- Olivia George, undergraduate student (Chemical Engineering), graduation in May 2019; this project is a part of her training and research for her departmental honors thesis, it has also helped her develop her scientific communication skills through conference presentation and journal publication
- Erin Conway, undergraduate student (Chemical Engineering), graduated in Dec 2017; she has gained expertise in multiple hands-on laboratory skills (e.g., nanomaterial synthesis, material characterization techniques), project leadership, team work, scientific writing, and conference presentation through this project
- Cody Flowers, undergraduate student (Chemical Engineering), graduated in May 2018; the project helped him gain experience in different nanomaterial synthesis, applications, independent research and method development. Cody is currently working as an engineer at Collider Tech in Chattanooga

Community and Broader Impacts

The proposed computational model will form the starting point to predict physiologically appropriate and patient-specific accumulation and flow velocity of specific nanodrugs, beyond the capabilities of current experimentation. This will be highly beneficial to the community in terms of cost-effective and faster development and screening of a more efficient nanoparticle-based drug that can serve as both a diagnostic and a therapeutic agent. There is an immense potential for product commercialization. In addition, the research project will also serve to train graduate and undergraduate students in cutting-edge research techniques.

Work products reduced to practice; provide a bibliographical entry where appropriate

This research has resulted in one published article, one publication in submission, three external conference presentations, and two internal conference presentations. Patent application related to the products from this research is currently being pursued by the P.I. and co-P.I.

Publications:

1. **Palchoudhury, S.;** Jungjohann, K.; Weerasena, L.; **Arabshahi, A.;** Gharge, U.; Albattah, A.; Miller, J.; Patel, K.; Holler, R. “Enhanced legume root growth with pre-soaking in α-Fe2O3 nanoparticle fertilizer” RSC Advances 2018, 8(43), 24075-24083. Refereed journal, impact factor: 2.936
2. **Palchoudhury, S.; Arabshahi, A.**; Gharge, U.; Albattah, A.; George, O.; Foster, Y. “Integrated Experimental and Computational Fluid Dynamics Approach for Nanoparticle Flow Analysis” Journal of Magnetism and Magnetic Materials, in submission. Refereed journal, impact factor: 3.046

External Conferences:

1. George, O.; Mcmahon, W.; **Arabshahi, A.; Palchoudhury, S.** "Synthesis and transport of Pt-iron oxide nanodrugs" National Council of Undergraduate Research Conference, Apr 2018 (Oral Talk)
2. Gharge, U.; Albattah, A.; McMahon, W.; Rayl, M.; Davis, E.; Arora, S.; Alp, K.; Flowers, C.; Patel, K.; Miller, J.; **Palchoudhury, S.** "Impact of engineered nanoparticles on seedlings" NanoBio Summit, Nov 2017 (Poster)
3. Gharge, U.; Albattah, A.; Patel, K.; Miller, J.; Conway, E.; Patrick, E.; George, O.; **Palchoudhury, S.** "Impact of engineered nanoparticles on seedlings" ACS SERMACS Nov 2017 (Poster)

Presentations at UTC:

1. **Palchoudhury, S.;** Al Hussain, Y.; Gharge, U.; Albattah, A.; **Arabshahi, A.** "Synthesis and transport of nanoparticle drugs", Technology Symposium, Apr 2018 (Poster)
2. George, O.; Patel, K.; Mcmahon, W.; Foster, Y.; Doumitt, C.; **Palchoudhury, S.; Arabshahi, A.** "Synthesis and transport of nanodrugs", Research Dialogues, Apr 2018 (Oral Talk)

New inventions reduced to practice and when they will be formally disclosed

The P.I. and co-P.I. are currently working in collaboration with SimCenter and UTC College of Engineering towards potential patents of two products from this research, as described below:

1. Increased growth of legumes using a drop of hematite nanoparticle fertilizer
2. Combined experimental and computational fluid dynamics approach to assess the transport of new Pt/Au-DNA-iron oxide nanodrugs

Outreach & Collaboration

The P.I. has been involved in teaching science at the SAT training workshop for high school students organized by UTC NSBE Student Chapter; location: on campus

Mentored one high school student in nanomaterials research in the P.I.'s laboratory at UTC; location: on campus

Established collaboration with Universities of Alabama and Buffalo and CINT, Sandia National Lab through this research

EXTERNAL FUNDING

Proposal Submissions

1. "A New Class of Penternary Chalcogenide Nanocrystals and Thin Films for Solar Energy Conversion Applications" submitted for Oak Ridge Associated Universities Ralph E. Powe Junior Faculty Enhancement Grant, $10,000
2. "Understanding the Effect of Engineered Nanoparticles in Agriculture" submitted for the Center for Integrated Nanotechnologies User Proposal, Sandia National Laboratories

Contracts/Awards Received

Center for Integrated Nanotechnologies User Proposal, Sandia National Lab
Type: Umbrella Non-Proprietary User Agreement

Sponsored Program Capacity Building Activities

Attendance and meeting with program officers at 2018 NIH Regional Seminar & Pre-Seminar Workshops - Washington, DC

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

We will look to become one of the pioneer research groups in computational and experimental evaluation of nanomedicine and drug delivery through continued publication in the field, presentations, and patent development. The *in silico* method developed through this research for analysis of nanoparticle transport through the body is a first of its kind in terms of application. Therefore, we will further develop the technique and potentially begin a new branch of research for nanomedicine.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

We will continue research in the field of health and biomedical applications related to exploratory nanodrugs for chemotherapy and development of an *in silico* model for flow of nano and micro-scale therapeutics through human pulmonary airway.

Interdisciplinary research in emerging areas of nanomaterials for supercapacitors and photovoltaics, material characterization of bio-inspired soft materials, and nanomaterials for sustainable agriculture will also be pursued by the P.I. and co-P.I. External collaborations will be pursued with Erlanger, Sandia National Lab, The University of Alabama, and University of Buffalo.

Tell us anything else we should know about this work not described above.

A key goal achieved through our project was the integration of computational methods with experimental results to answer a fundamental question of drug development and screening.

What barriers (if any) do you face to reach these next goals?

Access to different characterization tools like the transmission and scanning electron microscopy, atomic force microscopy, x-ray diffraction spectroscopy, and hyperspectral imaging for experimental investigation of the material properties of new nanoparticles synthesized at the P.I.'s lab may be challenging. We will address this through collaboration with the Universities of Alabama and Buffalo and through user proposals with Oak Ridge and Sandia National Laboratories. We will also look to write a major research instrument acquisition (MRI) grant.

FINANCIAL ACCOUNTING

Total Award Amount: $99,221.00

Cumulative Expenditures: $98,665.46

Remaining Award Amount: $555.54

Dr. Hong Qin, Lead PI

Co-PI(s): Dr. Craig Tanis
Other Personnel:
Postdoc: Haobo Guo. *Consultant:* Emine Guven

Project Title: "Connecting the Control Theory in Engineering to a Network Theory of Cellular Aging in Biology"

Date Submitted: 02/27/2017

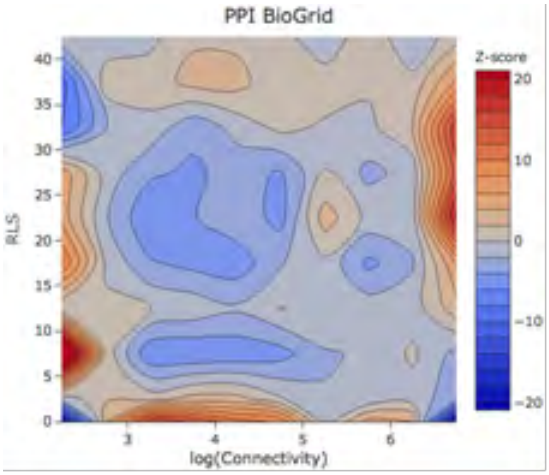
Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
Applying network theories in biomedical research is a promising approach in precision medicine. This project seeks to establish UTC as a national leader in an important new research direction on complex networks. With support of this project, we are prototyping a new algorithm for permutation of networks with power-law features that are found frequently in biology. This new network permutation algorithm enable us to reveal insights on the lifespan extension effect of calorie restriction. A manuscript is under preparation for network configuration analysis. This project has led to cross-discipline collaboration of dozens of faculty on UTC campus and multiple external grant applications.

Project Web Page(s):
Github repository are at https://github.com/QinLab

Connecting the Control Theory in Engineering to a Network Theory of Cellular Aging in Biology

Technology Area of Interest: Health and Biological Systems

PROPOSED TECHNICAL APPROACH	FINDINGS
• Develop computational tools • Perform large-scale data analysis	• Algorithm for network controllability analysis is prototyped in R • Algorithm for network configurational profiling is prototyped in R • High-performance computing of network permutation is prototyped and tested on SimCenter HPC clusters
RESULTS	**OTHER INFO**
 • PI Qin submitted an NSF REU proposal on August 23, "REU Site: ICompBio – Engaging Undergraduates in Interdisciplinary Computing for Biological Research". ~ $359K. This proposal is resubmitted on August 22, 2018. • Qin submitted a proposal, NSF IIS, "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education", ~$550K, on September 18, 2017. Funded. • NIH R15, subcontract, was submitted on Oct 25, 2017. Declined. • We have implemented a prototype code for network adjacency matrix analysis in R • A manuscript is in preparation for a high-impact journal. One manuscript has been accepted, and another one is under review.	**Budget and Schedule** Total Budget: $91,906.00 Actual Used: $91,905.08 Balance: $ 0.92 Total period of performance is 12 months. **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Software prototypes **Organization Information** UTC - SimCenter, Dr. Hong Qin 701 East M.L. King Boulevard Chattanooga, TN 37403 Telephone: 423-425-5492 Email: Hong-Qin@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

With support of this project, we are prototyping a new algorithm for permutation of networks with power-law features that are found frequently in biology. This new network permutation algorithm enable us to reveal insights on the lifespan extension effect of calorie restriction. A manuscript is under preparation for network configuration analysis. This project has led to cross-discipline collaboration of dozens of faculty on UTC campus and multiple external grant applications.

- PI Qin submitted an NSF REU proposal on August 23, "REU Site: ICompBio – Engaging Undergraduates in Interdisciplinary Computing for Biological Research". ~ $359K. This proposal is resubmitted on August 22, 2018.
- Qin submitted a proposal, NSF IIS, "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education", ~$550K, on September 18, 2017.
- NIH R15, subcontract, was submitted on Oct 25, 2017
- We have implemented a prototype code for network adjacency matrix analysis in R
- A manuscript is in preparation for a high-impact journal. One manuscript has been accepted, and another one is under review.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Postdoc interview and hiring.	Completed in July 2017.
Prototype software for network and controllability analysis	A graph permutation algorithm for power-law networks was prototyped. A prototype adjacency matrix based network analysis was written in R.
Application of network analysis to yeast network model of aging.	A manuscript on network model of aging was submitted to BMC Systems Biology in July 2018. Another manuscript on the network permutation is under preparation for Nature Methods.

Challenges & Strategies Used to Address / Overcome:

We had trouble to implement a GPU-based network analysis using adjacency matrix. We decided to use an alternative approach to implement the algorithm.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

We initially implemented a prototype code for network adjacency matrix analysis in C++. We decided to discontinue this effort and switch to R code development mainly due time constraint.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

This project enabled collaboration of at least 15 faculty from 5 departments at UTC, and collaboration with 10 faculty from three other universities and colleges.

Students Impacted

Brittany Campbell/Thomas is an undergraduate researcher worked on this project. She presented her research on UTC Research Day. She entered graduate school at UTHSC to pursue a PhD degree.

Community and Broader Impacts

None.

Work products reduced to practice; provide a bibliographical entry where appropriate

Peer reviewed journal publications:

1. Guven E, Qin H. The effect of Gaussian Noise on maximum likelihood inference of survival curves: A comparison of the Weibull and Gompertz models. Experimental Aging Research. Accepted.
2. QIN, H, Estimating network changes from lifespan measurements using a parsimonious gene network model of cellular aging. Submitted to BMC Systems Biology.

Outreach & Collaboration

We collaborated with colleagues from West Virginia University, Spelman College, and Tuskegee University.

EXTERNAL FUNDING

Proposal Submissions

Five submissions for external grants were made.

1. PI Qin submitted an NSF REU proposal on August 23, 2017, “REU Site: ICompBio – Engaging Undergraduates in Interdisciplinary Computing for Biological Research”. ~ $359K. This application was declined, but was encouraged for resubmission for revisions.
2. Qin submitted a proposal, NSF IIS, “Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education”, ~$550K, on September 18, 2017. This grant was funded on September 14, 2018.
3. An NIH R15, subcontract, was submitted on Oct 25, 2017. Declined.
4. An NSF Rule of Life letter of intent was submitted in January 2018. Declined.
5. NSF REU was revised and resubmitted on August 22, 2018.

Contracts / Awards Received

NSF IIS, “Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education”, ~$550K, was funded on September 14, 2018.

WHAT’S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

We plan to have at least 2 more manuscripts submitted in the near future.

What other related research will you pursue (and with whom) in light of the support you’ve received from CEACSE?

We are planning for a NIH R21 or R15 grant.

What barriers (if any) do you face to reach these next goals?

The funding period is not aligned with the graduate student support schedule.

FINANCIAL ACCOUNTING

Total Award Amount: $91,906.00

Cumulative Expenditures: $91,905.08

Remaining Award Amount: $0.92

Dr. Donald R. Reising, Lead PI

Co-PI(s): Dr. T. Daniel Loveless
Other Personnel:
Graduate Students: Ahmed Ibrahim, Bharat Patel

Project Title: “Unlocking the Secrets of RF-DNA Fingerprinting”

Date Submitted: 02/27/2017

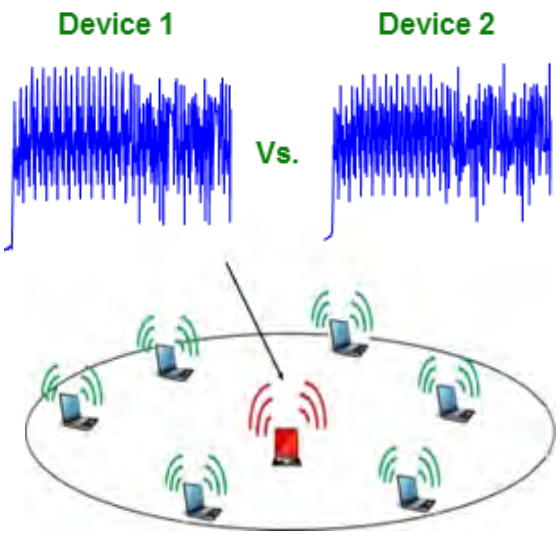
Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
The original focus for this effort was to investigate the connection between the waveform distinct and native attributes exploited by the RF fingerprinting process, and the hardware components that form a wireless device’s RF front-end. The goals of the project were to: 1) identify an individual or set of salient features by which to discriminate individual device from a much larger population and 2) select and/or develop hardware component models that capture variation(s) of RF front-end components. After award, the focus of the effort was slightly changed based upon a Broad Agency Announcement (BAA) from the Defense Advanced Research Projects Agency (DARPA). This BAA titled “Radio Frequency Machine Learning Systems (RFMLS)” was focused on the development of a comprehensive approach to developing a machine learning process by which to conduct Specific Emitter Identification (SEI) under various channel conditions and for the case of 10, 100, and 1,000 or more transmitters. In addition, DARPA was interested in the ability to “enhance” transmitter features to ease the process of SEI. Due to the nature of this BAA, Drs. Reising and Loveless teamed up with Pacific Northwest National Laboratory (PNNL) and submitted a proposal under Task 1 – Radio Frequency (RF) Forensics. The UTC team was responsible for Task 1B – RF Waveform Synthesis and PNNL would cover Task 1A – RF Feature Learning. The submitted proposal was not selected for funding; however, based upon feedback from the program officer the focus of the effort was shifted to the generation of preliminary results associated with Task 1B. The purpose of this is to facilitate a resubmission of the proposal to another Department of Defense (DoD) agency. Even with this change the project advanced the SimCenter’s work within the area of Urban Science and Technology by looking for a comprehensive and effective means by which to authenticate transmitters and enhance wireless security within IoT. IoT is critical to the “Smart City” initiative within Urban Science and Technology.

Project Web Page(s):
N/A

Unlocking the Secrets of RF-DNA Fingerprinting

Technology Area of Interest: Urban Systems and Defense

PROPOSED TECHNICAL APPROACH	FINDINGS
Task 1: Assess the Impact of Enhanced Features on Packet Error Rate (PER) • Two Assessments: Unmodulated Carrier Signal & Modulated Carrier Signal via Phase Modulation • Fixed Frequency & Changing Modulation Index • Fixed Modulation Index & Changing Frequency Task 2: Manipulation of CFO in Hardware Silicon Labs Si535x Evaluation Board • Two Cases: Unmodulated Carrier Signal & Modulated Carrier Signal	• Connect RF-DNA Fingerprint Feature(s) to Transmitter's RF Component(s) • Develop and Implement Feature Enhancement: How to Enhance, e.g., Phase Modulation of Transmitter's Local Oscillator Signal; Ease and Feasibility of Enhancement; Impact of Enhancement; Demodulation vs. RF-DNA ID • Creation of an Organic Software Defined Radio Capability, leveraged within Curriculum to Facilitate Experience based Learning and Current and Future Research • Enhancement of Inherent RF-DNA Fingerprint Features, that does not decrease demodulation performance and allows easier Identification of Radio using "Enhanced" Features
RESULTS	**OTHER INFO**
	**Budget and Schedule** Total Budget: $88,998.00 Actual Used: $88,998.00 Balance: $ 0.00 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-12 Task 3: Months 3-12 Task 4: Months 4-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work **Organization Information** University of Tennessee at Chattanooga Dr. Don Reising & Dr. Daniel Loveless Phone: 423-425-4225; Fax: 423-425-1732 Email: Donald-reisnig@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The re-focusing of the effort led to the reduction in the number of this project's tasks from three to two. The two tasks were developed directly based upon our proposal that was submitted in response to the DARPA BAA. In our proposal, we addressed Task 1B using the enhancement of IEEE 802.11a Wi-Fi transmitters through the intentional manipulation of their carrier frequency via the Local Oscillator (LO). Specifically, manipulation of the carrier frequency was to be achieved through frequency or phase modulation of the LO's reference clock signal. The desired outcome would be the enhancement of the Carrier Frequency Offset (CFO) feature. CFO is defined as the frequency difference that is present between the carrier frequencies created by the transmitting and receiving radios' LOs. The enhancement of the CFO feature was directly motivated by two factors: 1) prior, published work has successfully demonstrated a direct link between CFO and transmitter identification performance via RF-DNA fingerprints [1], and 2) the DARPA BAA specifically stated the custom tailored/enhanced waveform, "must successfully convey the intended information at a nominal rate" [2]. Basically, this DARPA requirement meant that any transmitter enhancement could not interfere nor reduce the ability of the transmitted information from being recovered by the receiving device. This had to hold even for the case of a commercial-off-the-shelf (COTS) device that was completely unaware of the enhancement, i.e., a COTS Wi-Fi's demodulation performance of the "enhanced" waveform should be the same as an unenhanced waveform. The tasks for the re-focused effort were:

Task 1: Assessment the Impact of CFO Manipulation on IEEE 802.11a Wi-Fi Demodulation

This task was focused on assessing whether or not the manipulation of the CFO feature would negatively impact the demodulation of the enhanced waveform by a COTS receiver. This task was performed using modeling and simulation in MATLAB®. The impact of the enhanced waveform on demodulation, via a COTS receiver, was assessed using Packet Error Rate (PER). The PER was calculated by dividing the number of error packets, after forward error correction, by the total number of packets received [3]. Ideally, the PER of a real communications system would be equivalent to that of its theoretical counterpart. In our case, the goal was for the PER associated with enhanced waveforms to match the case when standard, i.e., unenhanced, waveforms were received. Enhancement of the waveform was achieved through the manipulation of the carrier signal using Frequency Modulation (FM). The resulting carrier signal was then multiplied with the generated, complex, and baseband IEEE 802.11a Wi-Fi waveform to simulate up-conversion to bandpass. The enhanced, bandpass Wi-Fi signal is given by,

$$s(t) = x(t) * c(t), \tag{1}$$

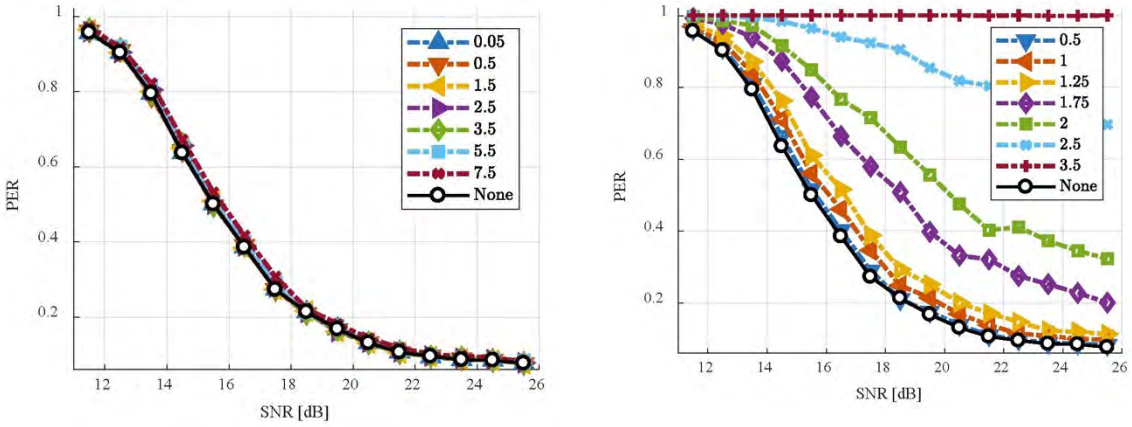
where $x(t)$ is the complex, baseband Wi-Fi signal,

$$c(t) = e^{-j\left[2\pi f_c t + \beta \sin\left(2\pi f_m t\right)\right]}, \tag{2}$$

is the carrier signal, f_c is the LO output signal's frequency, β is the modulation index, and f_m is the frequency of the enhancing signal. In this task a sinusoidal signal was used to enhance/manipulate the carrier signal's frequency, but other signal types can be used in its place, e.g., square wave. The simulation was performed using a Rayleigh channel fading model with average path gains, $g \in [-4.9, -20.9]$, and path delays, $d \in [0, 1{,}760] \times 10^{-9}$, to represent a large open space environment with a root mean square (rms) delay spread of 250 ns [4]. The maximum allowable Doppler shift was set to 50 Hz and an arbitrary delay of 5 μs added to account for all possible channel profiles. The analysis was conducted for signal-to-noise ratios (SNRs) from 11.5 dB to 25.5 dB in 1 dB steps. For a given SNR, the simulation was terminated when either the total number of packet errors or transmitted packets reached 1,000 or 10,000, respectively. Using the above parameters and settings two different PER analysis cases

were performed using a: 1) fixed modulation frequency f_m and changing modulation index, and 2) fixed modulation index and changing modulation frequency.

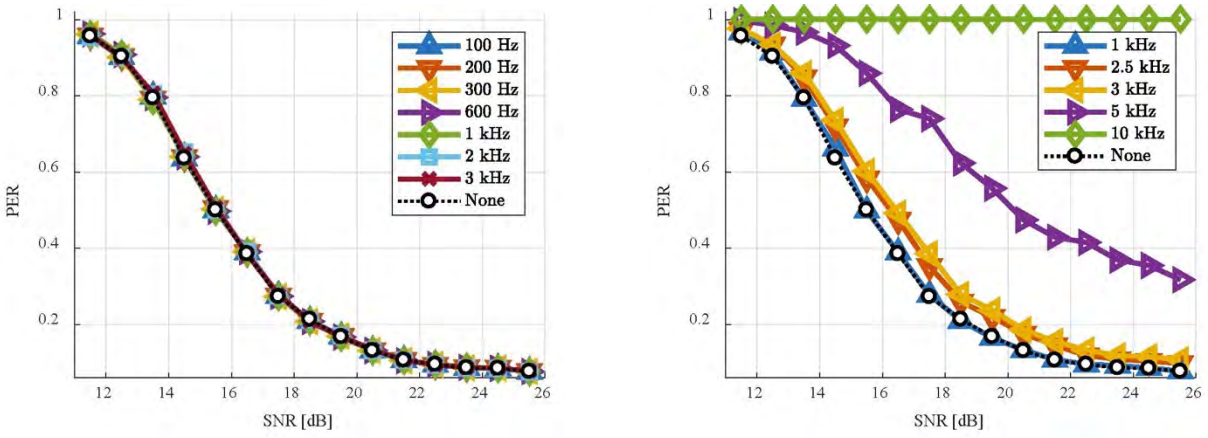
Figure 1 presents PER performance curves associated for a modulation frequency of 1 kHz (Fig. 1a) and 10 kHz (Fig. 1b) for $\beta \in [0.05,\ 7.5]$. For the f_m=1 kHz case the PER performance does not change even for large values of β, Figure 1a. However, when the modulating frequency f_m=10 kHz, the PER performance begins to degrade for $\beta \geq 1$; thus, suggesting a restriction to narrowband FM, i.e., $\beta \ll 1$.



(a) FM frequency of 1 kHz. **(b) FM frequency of 10 kHz.**

Figure 1. Packet Error Rate performance for a fixed FM frequency and changing β.

The PER performance curves associated with changing modulation frequencies, $f_m \in [0.1,\ 10]$ kHz, and a fixed modulation index of β=0.5 and β=3.5 are shown in Figure 2a and Figure 2b, respectively. For β=0.5 the modulation frequency can get as high as 3 kHz without negatively impacting the PER performance. If the results in Figure 1b are taken into consideration, then a modulation frequency as high as 10 kHz will not adversely affect the PER performance. However, when β=3.5, as shown in Fig. 2b, the PER performance is adversely impacted for $f_m \geq 1$ kHz.



(a) Modulating index of β = 0.5. **(b) Modulating index of β = 3.5.**

Figure 2. Packet Error Rate performance for a fixed β and changing modulating frequency.

The PER performance curves presented in Figure 1 and Figure 2 suggest that the values selected for the modulation index and frequency must be chosen carefully if one does not want to negatively impact the receiving device's PER. If narrowband FM ($\beta \ll 1$) is selected, then the modulation frequency can be rather large without sacrificing PER performance. If narrowband FM is not selected, then careful selection of the modulation frequency f_m must be observed. However, degradation of PER may be advantageous if identification of a particular transmitter is necessary. This could be a temporary state when first joining the wireless network or periodically throughout operation to perform validation of a given transmitter's/device's identity. During these periods a brief degradation of PER may be acceptable to perform authentication of a device to improve overall network security.

The use of Modeling & Simulation (M&S) does make it possible to perform simulated manipulation of previously collected Wi-Fi signals for identification of the devices using the RF-DNA fingerprinting process. This would simply require the estimation and removal of CFO, as in [1], followed by simulated manipulation of the CFO using (1). However, this was not done as part of this effort, because such an approach would neglect the impact of additional coloration that would be imparted by the physical RF front-end components that come after the mixing stage. Thus, neglecting any additional interactions that may be exacerbated by the carrier signal's manipulation. This task did provide invaluable insight into the selection and interaction of the chosen modulation index and frequency values that will be used for subsequent hardware implementation.

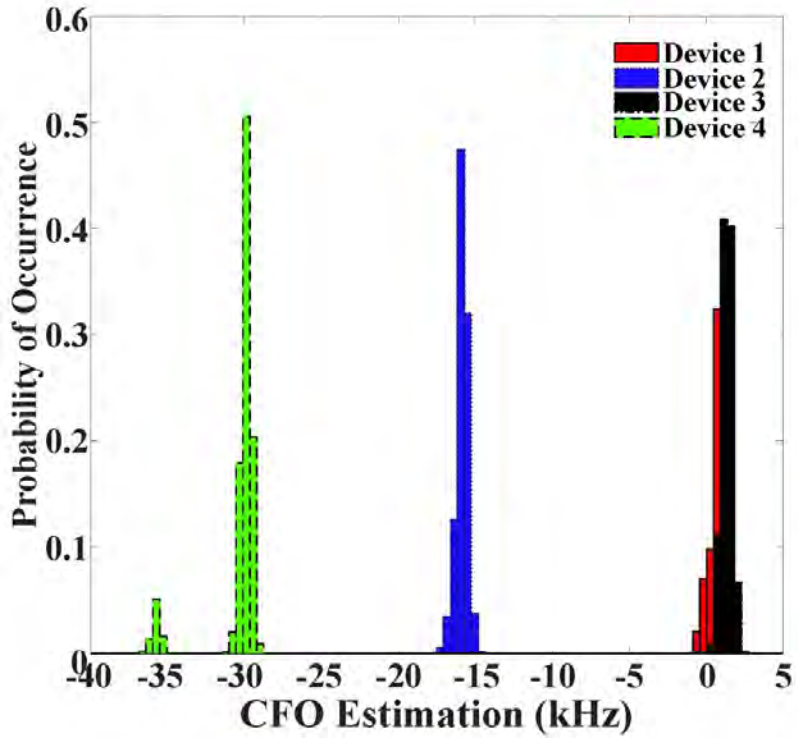


Figure 3. Probability Mass Functions of CFO values estimated from the signals collected from four Wi-Fi radios [1].

Task 2: CFO Manipulation in Hardware

This task was aimed at establishing the first direct connection between waveform classification performance and the features attributed to the Local Oscillators (LOs) of the transmitting and receiving radios, thus enabling enhancement of the CFO feature of a waveform. Figure 3 shows the Probability Mass Functions (PMFs) associated with the CFO values estimated from the collected waveforms of the four Wi-Fi radios [1]. The four Wi-Fi radios' signals were collected using the same receiver; thus, differences in the estimated CFO values are attributed to the LO of the corresponding transmitter. Even for the case of multiple receivers, the CFO values within a specific set of received waveforms will contain the same receiver LO bias, thus enabling the ability to learn this common bias. It is important to note that the shape of each PMF represents the behavior of the transmitter's LO with respect to that of the receiver's LO over time, because each CFO value was estimated from a new, consecutive transmission. Thus, we establish three definitions, which are key to our approach:

a. *Characteristic*: A singular measurement associated with specific component within the RF front-end.

b. *Feature*: A singular measurement of the RF waveform, e.g., the CFO value.

c. *Behavior*: Learned through the observation of a given feature over time, e.g. CFO values across transmissions from a specific radio.

Based upon the PMFs shown in Figure 3, the most challenging case of radio ID is when Device 1 and 2 represent the authorized (Alice) and rogue (Trudy) radios, respectively. This is because the distribution of Alice's and Trudy's intrinsic CFO features are quite similar in shape, spread, and measured values. As shown in [1], this resulted in these two devices being confused with one another by the selected machine learning (ML) algorithm. Thus, presenting the possibility for Trudy to gain unauthorized network access by posing as Alice. Firstly, the work in [1] did not consider the behavior of Alice's and Trudy's intrinsic CFO feature, thereby ignoring another potential dimension by which to differentiate Alice from Trudy. Secondly, for Trudy to completely pass as Alice would require the two associated PMFs to be identical. The fact that they are not illustrates the difficulty faced by Trudy to pose as Alice in all cases. For Trudy's PMF to match that of Alice's would require Trudy to have the ability to inherently overcome her own radio's intrinsic feature(s) and associated behavior(s). Lastly, the fact that these two PMFs are different presents a potential mechanism by which the trainable system (Bob) can separate Alice from Trudy. If Alice manipulates her LO in such a way that it is restricted in behavior to the CFO values associated with the non-overlapping portion, then Bob's ability to separate Alice from Trudy is enhanced without detrimentally impacting Bob's understanding of Alice's behavior nor the associated information rate of the implemented communications standard.

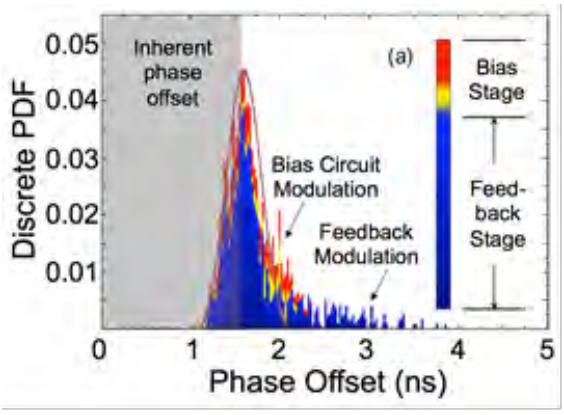
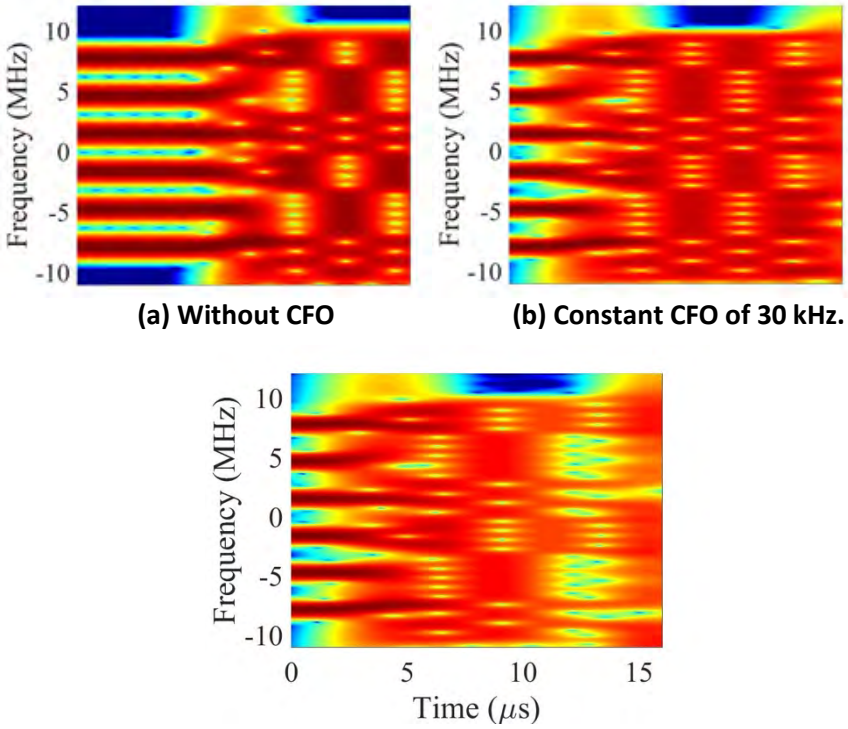


Figure 4. Phase offset and jitter of a local oscillator with current injection within the bias and feedback elements. The distribution of the inherent feature may be modulated without changing the fundamental behavior [5].

One approach that allows for unique variation of inherent features is the manipulation of the instantaneous frequency and phase of an LO, e.g., through modification of internal voltage or current levels. The work in [5] showed that the injection of photocurrent into various locations within the LO resulted in the modulation of the phase offset feature. The altered Probability Density Function (PDF), shown in Figure 4, captures the impact of the modulation on the phase offset and Gaussian *rms* jitter of the LO. Moreover, attributes within the altered PDF are specific to the type and location of current injection. Thus, presenting a novel means by which to enhance Alice's intrinsic features. Our approach is to allow Alice to adjust or modulate her behavior, e.g. the frequency and/or phase of the LO, within the allowable range of the selected communications standard, to ease identification through the altering of the CFO feature. This approach permits the tailoring of Alice's transmitted waveform, while maintaining consistency with the appropriate communicating standard to ensure conveyance of the intended information at the nominal rate.

LO manipulation was used to directly manipulate the transmitter's RF front-end components associated with the intrinsic signaling features. The behavior of the feature(s) was then used to determine the range of intentional manipulation that can be applied to the related RF front-end component(s) by the transmitter's ML algorithm. This permits enhancement of Alice's features without negatively impacting Bob's understanding of Alice's behavior as well as maintaining compliance with the associated communications standards to ensure nominal rate transference of information. Compliance with the selected communication standards is ensured through the integration of commercial off the shelf (COTS) radios within the communications network structures. The ability of COTS radios to receive and successfully demodulate an intentionally manipulated waveform will ensure compatibility with legacy and current communication devices and networks.



(a) Without CFO **(b) Constant CFO of 30 kHz.**

(c) Up-chirp CFO from 5 Hz to 40 kHz.

Figure 5. Time-frequency response of three IEEE 802.11a Wi-Fi preambles.

The basis of our approach is that if the behavior of Alice's CFO values are distributed the same as Device 4 of Figure 3, then Alice's LO can be manipulated to change frequency, within the range of [-28, -36] kHz, over the duration of a single transmission. In other words, instead of the trainable system, i.e., Bob, observing and exploiting an intrinsic constant CFO value associated with Alice; Bob will exploit a CFO feature that is changing over Alice's transmitted waveform. Figure 5 provides representative time-frequency illustration of the impact such manipulations can have on Alice's transmitted waveform. Figure 5(a) shows the time-frequency response of an ideal 802.11a Wi-Fi preamble in which there is no CFO present. Figure 5(b) represents one of Alice's preambles in which a constant CFO value of 30 kHz has been added to mimic the intrinsic feature. In Figure 5(c), the intrinsic CFO feature has been enhanced through the inclusion of a CFO value that is linearly increasing (i.e., up-chirp), from 5 Hz to 40 kHz, over the duration of the preamble. The enhancement of Alice's discriminatory feature is captured in the clear as well as subtle differences that can be seen between the transmissions in Figure 5.

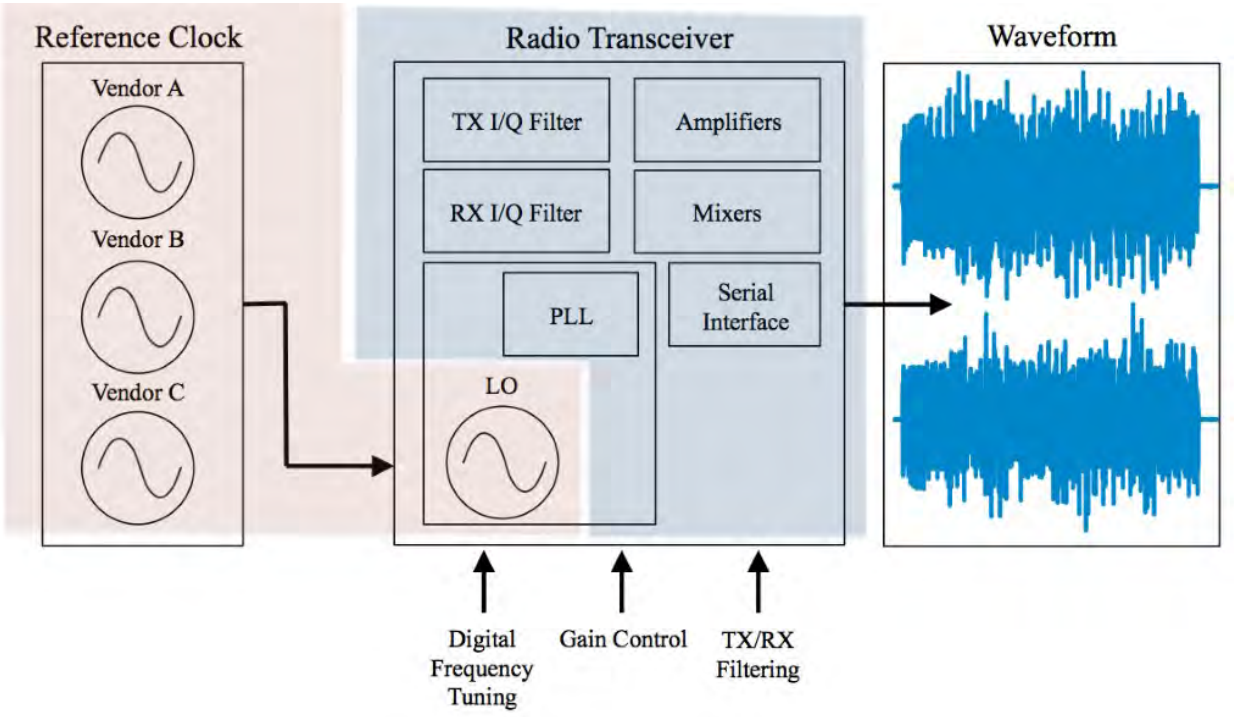


Figure 6. Block diagram showing behavior characterization of components of a COTS radio.

In order to establish the direct connection between hardware characteristics and inherent waveform features, we 1) characterized COTS oscillators and SDR transceiver peripherals, and 2) measured characteristic and enhanced SDR features. Figure 6 illustrates the approach for behavior characterization of components, and Figure 7 illustrates the hardware setup for measurement of the impact of LO modulation on the MAX2837 transceiver. Additional COTS experiments were designed for measurement of the Si5350 clock generator and HackRF One Software-Defined Radio. Experiments on each evaluation board indicate that an external modulated LO can be applied to vary the carrier frequency on the output port. Additionally, as shown in Figure 8, the spread in the frequency spectrum can be controlled via phase modulation. In Figure 9, phase modulation was injected into a 2.4 GHz WiFi carrier via the LO and resulted in a spread in the signal frequency spectrum within limits imposed by the standard. These results provide strong evidence of the feasibility of our proposed approach to

enhancement of IEEE 802.11a Wi-Fi transmitter security through the intentional manipulation of behavior.

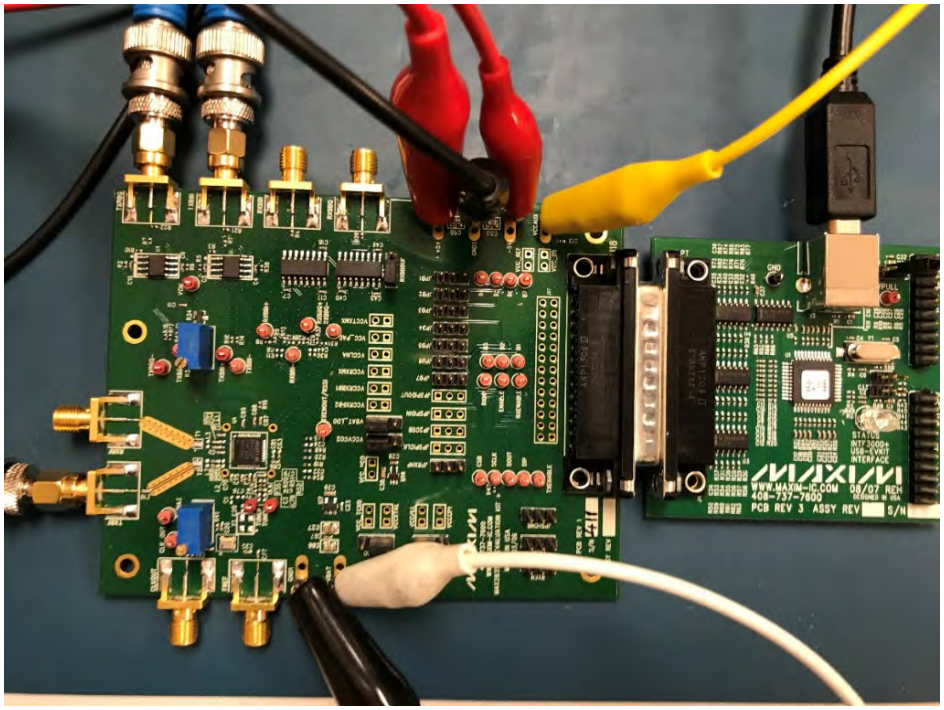


Figure 7. Hardware setup for measurement of the impact of LO modulation on the MAX2837 transceiver.

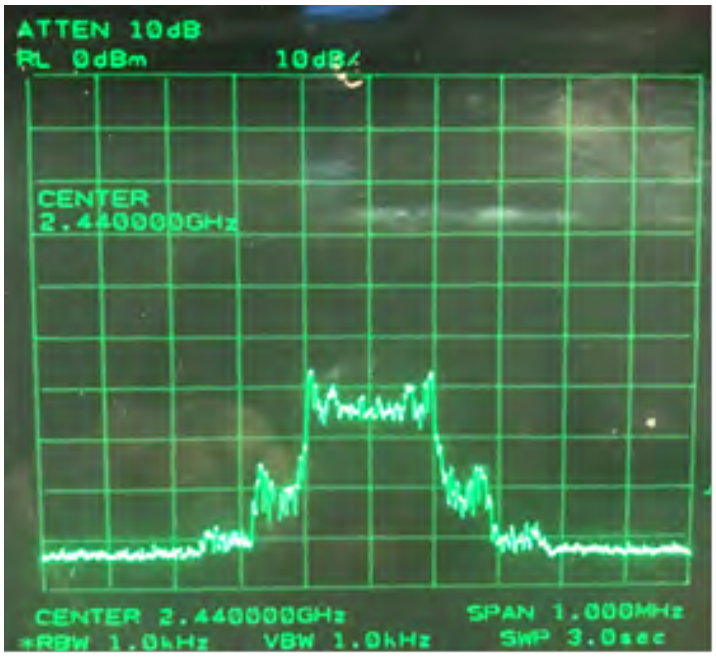


Figure 8. Output spectrum of the 2.4 GHz WiFi carrier generated by the MAX2837 with a phase modulated LO.

References:

[1] C. Wheeler and D. Reising, "Assessment of the Impact of CFO on RF-DNA Fignerprint Classification Performance," in International Conference on Computing, Networking and Communications (ICNC), Silicon Valley, CA, June 2017.

[2] DARPA Microsystems Technology Office, "Radio Frequency Machine Learning Systems (RFMLS)," Defense Advanced Research Projects Agency, August 11, 2017.

[3] S. Hanatani, T. Akita and I. Murata, " International Civil Aviation Organization (ICAO)," 5 June 2014. [Online]. Available: https://www.icao.int/safety/acp/ACPWGF/ACP-WG-S-Web%20Meeting%205/ACP-WG-S_WP04-ErrorMeasurment_r11%20%20(2).docx. [Accessed 16 July 2018].

[4] K. Haider and H. Al-Raweshidy, "HiperLAN/2 Performance Effect Under Different Channel Environments and Variable Resource Allocation," University of Kent, Cantebury, U.K., 2002.

[5] T. Loveless, L. Massengill, B. Bhuva, W. Holman, M. Casey, R. Reed, S.Nation, D. McMorrow, and J. Melinger, “A Probabilistic Analysis Technique Applied to a Radiation-Hardened-by-Design Voltage -Controlled Oscillator for Mixed-Signal Phase-Locked Loops,” IEEE Trans. Nucl. Sci., vol. 55, no. 6, pp. 3447-3455, Dec. 2008.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Assessment the Impact of CFO Manipulation on IEEE 802.11a Wi-Fi Demodulation	Successfully assessed the relationship between a combination of modulation index and frequency values using Packet Error Rate performance. The goal was to select values for these parameters in such a way as to not negatively impact the PER performance of a commercial off-the-shelf IEEE 802.11a Wi-Fi device that does not implement carrier signal manipulation as a means of enhancing device identification performance using RF-DNA fingerprint.
CFO Manipulation in Hardware	Established protocol for LO manipulation for CFO modulation. The Max2837, Si5350, and HackRF One commercial off-the-shelf (COTS) hardware was successfully used to demonstrate procedures and collect preliminary results.

Challenges & Strategies Used to Address / Overcome:

1) The timeline has been shortened due to late notification of award (June 2017); thus, we were not able to hire two students per the proposed budget and work. We will begin work using one of Dr. Loveless’ graduate assistants. He will be used to identify the appropriate platform and construct the testbed.

2) The primary technical challenge involved identification of a clear link between an RF front-end component and the resulting RF fingerprint. We reduced the scope of the problem, starting with the characterization of the impact of local oscillator (LO) variation on RF fingerprints. Previous work suggests the link between LO and RF fingerprint features is relatively clear.

What didn’t work? What did you disprove or learn from the parts that didn’t meet your initial concept at the proposal?

Initially, the project was officially kicked-off on July 1, 2017; however, the entire project was delayed by a full semester due to late notification of award. The prior year of CEACSE grant awardees were notified May 19, 2016, which provided ample time for the recruitment and hiring of the necessary graduate research assistants. For this CEACSE selection, awardees were not officially notified until June 15, 2017. This represented a delay in notification of roughly one month. This caused the loss of a vital window in which to recruit graduate researchers as most of UTC's recent graduates would have already accepted full-time positions. Also, the hiring of foreign students was missed, because these students require visas to work within the U.S. and have a strict application submission and approval timeline.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

PI: This award represents the first funding directed at furthering Dr. Reising's principle research interest: specific emitter identification via Radio Frequency-Distinct Native Attributes (RF-DNA) fingerprinting. This project facilitated the initial research into a specific feature that has been exploited to facilitate identification of IEEE 802.11a Wi-Fi transmitters [1]. It also led to the development and initial assessment of a process by which to manipulate/enhance that feature without negatively impacting the network's ability to transmit information. This project has provided Dr. Reising an initial set of Software Defined Radios (SDRs) that will be used in Dr. Reising's research and courses. For example, the SDRs purchased under this project will be used as part of a Senior Design Project in which the student will assess if a replay attack can be successful in thwarting the RF-DNA fingerprinting process, i.e., an unauthorized device records and plays back an authorized radio's waveform to gain access to the network. Dr. Reising will also use some of these SDRs to present the first Digital Communications Laboratory this upcoming fall semester. Lastly, this project provides a data set from which preliminary results can be generated for use in pursuing extramural funding.

Co-PI (Dr. Loveless): This effort has resulted in a direct connection between Dr. Reising's work in communications and RF security to Dr. Loveless' primary research area of extreme environment electronics. The connection has resulted in a broader application space to apply ongoing research findings and has allowed for the gathering of preliminary evidence for proposals in the areas of Urban Science, Communications, and Defense. Through this process, we discovered an untapped research area within Dr. Loveless' expertise of space and radiation effects in electronics which has already resulted in one conference presentation, a journal submission, and a follow-up CEACSE award in which we aim to explore the use of RF fingerprinting techniques and machine learning to aid in identification of radiation effects and reliability degradation.

Students Impacted

Ahmed Ibrahim: Mr. Ibrahim is seeking a Master's of Science in Electrical Engineering. Mr. Ibrahim conducted all of the work related to configuration of the HackRF One SDR to transmit and receive using the IEEE 802.11a Wi-Fi. This work has served as an introduction of Mr. Ibrahim to the RF-DNA fingerprinting process. Prior to this effort, Mr. Ibrahim had no experience with the using SDRs, specific emitter identification, nor the collection of wireless signals for later processing and research. This work has provided invaluable and necessary experience in scoping and conducting research. Such work requires the development of critical thinking and problem solving skills as well as transitioning from undergraduate to a graduate level of work, which are necessary for his Master's thesis research.

Bharat Patel: Mr. Patel is seeking a Master's of Science (M.S.) in Electrical Engineering. Mr. Patel assisted in the work related to the HackRF One SDR and established the initial CFO manipulation protocol using the Max2837 and Si5350 COTS. This work has linked to his M.S. thesis work on the use of RF-DNA fingerprinting for assessment of ionizing radiation

degradation (Ionizing Radiation Effects Spectroscopy), which has resulted in one conference presentation and a journal submission. This work has provided invaluable and necessary experience in scoping and conducting research. Such work requires the development of critical thinking and problem solving skills as well as transitioning from undergraduate to a graduate level of work, which are necessary for his Master's thesis research.

Community and Broader Impacts

The potential impacts of this project is the initial development of a process by which to enhance features to ease identification of a specific transmitter for use in augmenting wireless network security. The selection of IEEE 802.11a Wi-Fi was motivated by: 1) the significant amount of specific emitter identification research performed using this communications scheme, and 2) the use of OFDM or OFDM-based modulation schemes in fourth and fifth generation wireless communication standards such as: Long Term Evolution (LTE), 802.11ac, 802.11ad, 802.11ax, and Worldwide Interoperability for Microwave Access (WiMAX). The need for an effective, robust, and computationally simplistic approach to specific emitter identification is essential to creating and/or augmenting Internet of Things (IoT) and wireless network security as a whole.

Work products reduced to practice; provide a bibliographical entry where appropriate

None

Outreach & Collaboration

The DARPA proposal submission led to the creation of a collaborative research relationship with Pacific Northwest National Laboratory. This relationship continues as we generate preliminary results and subsequent resubmission opportunity.

Participated in the poster session of UTC's 2018 Research Dialogues. The poster was presented for both days of the event and Mr. Ibrahim stood by to address questions and general conversation in regards to the research.

The use of RF fingerprinting for the analysis of radiation degradation in RF circuits was presented by Bharat Patel at the 2018 Nuclear and Space Radiation Effects Conference in Kona, HI, and has resulted in a journal submission (currently in review) to the IEEE Transactions on Nuclear Science.

EXTERNAL FUNDING

Proposal Submissions

DARPA Microsystems Technology Office BAA: Radio Frequency Machine Learning Systems.
https://www.fbo.gov/index?s=opportunity&mode=form&id=496c944ced6a0434e613bee86a238a6c&tab=core&_cview=1
Dates: August 2017 - Release of RFP, October 2017 - Full proposal submitted, $2.7M

- Not selected for funding.

Southeastern Center for Electrical Engineering Education (SCEEE)
Dates: April 2018 - Release of RFP, July 2018 - Full proposal submitted, $24,833

- Not selected for funding.

U.S. Army Communications-Electronics Research Development and Engineering Command (CERDEC)
Space and Terrestrial Communications Directorate
Solicitation: BAA-18-R-STCD - Open call from 20 June 2018 to 19 June 2023

- Two step solicitation via white paper to determine interest.
- Possible opportunity for re-submission of the DARPA proposal. This proposal would contain preliminary results generated using the resources, lessons learned, processes, and techniques investigated under this CEACSE grant.

Contracts / Awards Received

None

Sponsored Program Capacity Building Activities

Participation in the inaugural "Military IoT and Sensors Summit" in Alexandria, Virginia from 15-16 May 2018. Dr. Reising attended the summit to get a better sense of the challenges as well as opportunities for the application of RF-DNA fingerprinting within DoD IoT applications. Participation in this summit resulted in Dr. Reising making connections with two people: 1) Glenn Kesselman from Kesselman & Associates: Cyber Security Products & Services, and 2) Dr. Stephen Russell from Army Research Laboratory's Battlefield Information Processing Branch. A summary of the developing and ongoing relationship with these two individuals follows.

- Meeting Mr. Kesselman has directly led to Dr. Reising being introduced to Rosetta Cyber Systems. Rosetta Cyber Systems is a technology company developing solutions for industrial IoT systems and applications. This introduction has resulted in Mr. Doug Gisby coming to UTC to learn more about the smart building and IoT research being conducted by Drs. Reising, Sartipi, and Loveless. Mr. Gisby expressed Rosetta's interest in conduction a pilot study within the smart building testbed due to be developed and deployed within the SimCenter. Rosetta Cyber Systems is willing to give UTC a copy of their software at no charge as well as access to the data. This represents a significant opportunity for collaboration with industry and growth of our smart building research.
- Dr. Russell is the Branch Chief of ARL's Battlefield Information Processing Branch and has a vested interest in the development of "Internet Battlefield of Things" (IBoT). This includes research and development of IBoT security mechanisms and techniques. He presented the idea and associated challenges at the summit. Currently, Dr. Reising has an ongoing discussion with Dr. Russell over email. We are currently coordinating either a phone or face-t-face meeting. Per Dr. Russell's request, Dr. Reising has shared with him his current MILCOM conference paper that is under review. Dr. Reising will continue to correspond with Dr. Russell in hopes of establishing a source of collaboration and funding of continued work within the area of IoT security using RF-DNA fingerprinting.

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

We are actively looking for possible research funding opportunities. One such opportunity is the open BAA released by the U.S. Army CERDEC (BAA-18-R-STCD). Additionally, there is potential for funding through the NSF's Cyber Physical Systems (CPS) call. The long term goal is the development of a robust wireless network security mechanism based upon RF-DNA fingerprinting that augments and coordinates with other network security mechanisms, e.g., encryption, block chain, etc. The work conducted here is ongoing and will be integrated as well as extended within Master's thesis research. Specifically, Mr. Ahmed Ibrahim is conducting research to test the developed approach within Software Defined Radios (SDRs). This will allow for testing of the technique in enhancing wireless device identification while not or minimally impacting the demodulation process. Testing within actual hardware is necessary to assess how the enhancement is affected by other "downstream" components within the transmitter's RF front-end. For instance, how does the amplifier change the enhancement prior to transmission if at all? Beginning in the fall semester of 2018, preliminary research will be conducted in determining the scale of RF-DNA fingerprinting, i.e., how many devices can be effectively discriminated. This work will be conducted as part of a Ph.D. dissertation conducted by Mr. Mohammed Fadul. The results of this research will serve as preliminary results that can be integrated within a follow-on proposal.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

This CEACSE award is part of a much larger project that Dr. Reising has envisioned for the further development of specific emitter identification based wireless network security. The preliminary results that will be generated using the data set(s) created under this effort will be combined with recent RF-DNA fingerprinting multipath channel work completed as part of an extramural funding proposal targeting the Department of Defense. The U.S. Army has a vested interest in the development of the Internet of Battlefield Things; thus, there is strong interest in network security as well as exploitation. This grant also afforded Drs. Reising and Loveless to see a direct connection between their respective research interests and efforts. It has directly led to the development of the Ionizing Radiation Effects Spectroscopy (IRES) approach that has demonstrated initial success in radiation effects analysis (journal paper currently under review). IRES is based upon RF-DNA fingerprinting and provides the first non-invasive approach for measuring total-ionizing dosage in arbitrarily complex circuits. This initial IRES work led to the submission and successive awarding of a 2018-2019 THEC CEACSE grant focused on furthering the IRES concept. This CEACSE award also afforded Drs. Reising and Skjellum to discuss points of collaboration for IoT security. More specifically, the idea is to combine the concept of RF-DNA fingerprinting with that of blockchain by replacing/augmenting the Physically Unclonable Function (PUF).

Tell us anything else we should know about this work not described above.

This work actually served a critical role in creating an organic capability for conducting SDR-based research. This research is not limited to just RF-DNA fingerprinting, but also other wireless communication research. For example, this project has spurred collaborative research with Dr. Sartipi within the area of 5G communications, which has been targeted as one scheme necessary for IoT and Smart City/Community development. As alluded to above, this project is fostering undergraduate research and learning within the areas of wireless communications and RF-DNA fingerprinting.

What barriers (if any) do you face to reach these next goals?

This largest challenge is finding a sponsoring agency interested and willing to fund ongoing work within this research area. Dr. Reising has begun looking and fostering relationships within the DoD as well as industry through his participation in seminars, workshops, and conferences. In particular, Dr. Reising will be attending the 2018 Military Communications (MILCOM) conference this coming October. This conference is attended by DoD, federal agencies, as well as industry partners; thus, it affords Dr. Reising an excellent opportunity to foster the needed relationships necessary to continuing this work.

FINANCIAL ACCOUNTING

Total Award Amount: $92,062.00

Cumulative Expenditures: $91,901.98

Remaining Award Amount: $160.02

Dr. Mina Sartipi, Lead PI

Co-PI(s): Dr. Farah Kandah
Other Personnel:
Post-doctoral fellow: Khashayar Kotobi, *Graduate student:* Steven Schmitt, *Undergraduate students:* Dylan Brownell and Peyton Ball

Project Title: "Enabling Wireless 3C Technologies for Smart and Connected Cities"

Date Submitted: 02/27/2017

Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
We propose using edge computing and caching to enhance wireless communications in terms of bandwidth and delay by leveraging concept of mobile 3C systems (communications, computing, and caching (i.e., 3C)). First we argue that without leveraging concepts of edge computing and caching, the huge burden of data transmission and processing necessary for smart city applications and concept is going to exhaust the current wireless infrastructure. Then we demonstrate the need to merge edge computing with caching to enhance wireless communication needed for massive data collection in smart cities. To address the security concerns of using IoT in smart cities, we propose using a blockchain database to secure communication between the smart city and home devices and sensors. This will provide the scalability that is necessary for data transfer between the massive numbers of nodes in IoT that current security protocols do not provide.

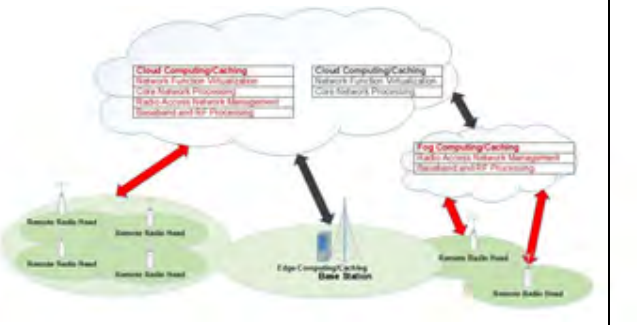
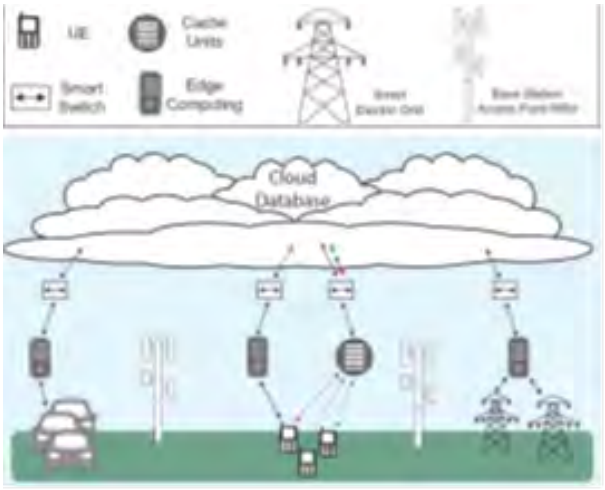
The project also focuses on creating a dynamic solution using Software-Defined Networking to meet network needs in supporting high traffic demand. We work on developing a Smart and adaptable network design seeking to utilize network resources more efficiently by identifying traffic patterns and analyzing network metric to dynamically build virtual slices. With this design, we were able to minimizing packet loss, maximizing network link utilization, and efficiently reduce the load on the controller. To support the SimCenter efforts in the field of Urban System, our team worked on developing an SDN testbed as a proof of concept that can be adopted on a larger scale. The broader impact of this project is its ability to be adopted in different fields in smart cities setups.

Project Web Page(s):

- https://github.com/fkandah/2018---Software-Defined-Network-Testbed
- https://github.com/khashi86/CCC

Enabling Wireless 3C Technologies for Smart and Connected Cities

Technology Area of Interest: Computer Networks

PROPOSED TECHNICAL APPROACH	FINDINGS
• For caching units, giving frequent access to popular content that is cached at local access points, roadside units and base stations have been introduced to encounter growth in mobile traffic. • For edge computing units, implementing edge computing units in specific locations to reduce the transmission delay. • For Blockchain security protocol, the number of wireless users that IoT and smart city applications are required to have wireless connection to the edge computing units is huge and as a result the current secure protocols cannot be used since they are not scalable. • Developed a dynamic and adaptable routing scheme over SDN to enable the network to handle extra demand on traffic and efficiently using the available resources.	• Caching units • Edge computing units • Blockchain security protocol • Software-defined networking 
SCHEMATIC	**OTHER INFO**
	**Equipment to be Used** Total Budget: $92,000.00 Actual Used: $79,407.00 Balance: $ 12,592.00 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • The Code and the manual will be posted on GitHub and will be provided upon request. **Organization Information** UTC, Dr. Mina Sartipi 615 McCallie Ave. Chattanooga, TN 37403 Telephone: 423-425-4225 Email: mina-sartipi@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

We provided a design paradigm for 3C service deployment, placement, and migration in this project. By Moving computing and caching units from the cloud to the edge which is closer to mobile users, we showed that network designers can greatly reduce service latency and improve the network quality of service. We also showed that Service deployment and placement decide how to allocate 3C resources for a mobile application at the service admission while service migration deals with seamless handover of wireless communications and dynamic migration of computing/caching components as the corresponding user moves across different geographical areas.

Our research finding shows that employing caching and edge computing units in future smart and connected cities development will drastically improve the functionality of current wireless infrastructure. This is done by modeling the wireless communication as a multi variable optimization problem. Here by focusing on caching to alleviate the bandwidth shortage and edge computing to reduce the delay, we can optimize the performance of our wireless network based on the quality of service required for different applications.

Our study shows that implementing edge units can drastically save the communication time when the number of wireless users increases. This will improve the quality of service for many real-time applications that are sensitive to delay and growing in number (for example, autonomous vehicles). By using the hybrid scheme, city developers have a trade-off between the number of edge computing units deployed and the mobile traffic. Our findings also shows that power consumption increases when we employ our technique when the number of mobile users increases. Saving in terms of power consumption is not as drastic as delay since after edge computing units, most data transmission is on wired transmission.

Co-PI's research seeks to develop an SDN system that uses metric-based analysis to virtually and automatically slice our network. These virtual slices will group hosts based on network activity aiming for efficient use of network resources. Our goal, by dynamically slicing the network based on metrics such as link utilization and packet drop rate, is to create an intelligent and adaptable network design that outperforms traditional methods.

With the proposed design, we were able to improve the network performance through minimizing packet loss, maximizing network link utilization, and efficiently reduce the load on the controller.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
• Improve the wireless network quality of service in terms of delay and bandwidth by employing edge computing for delay sensitive applications and caching for applications with a high demand for bandwidth to adapt the current wireless technology for smart city development. • Define a multi variable optimization problem for applications that have both delay and bandwidth constrains and	• We merged caching and edge computing units to improve the wireless network performance and enhance the quality of service offered for smart and connected cities applications. • We provided security by employing blockchain data base that is scalable in contrast to the current wireless security protocols that are not scalable for IoT nodes that are going to be used for

merging the edge computing and caching units to address the quality of service requirements for wide • Improve the connectivity in the network, allow the network to utilize its resources and be able to handle the traffic more efficiently. • Substitute the need to use hardware solutions to overcome load balancing issues in the network.	implementing the applications necessary for smart and connected cities. • We were able to automate the network utilization process by developing a dynamic and adaptable network design over software-defined network that allow the network to dynamically handle the traffic and balance the load in the network.

Challenges & Strategies Used to Address / Overcome:

Blockchain technology has been used to address the scalability issues facing massive increase in terms of nodes and applications that are going to be connected in a smart and connected smart city.

Traffic engineering and pattern recognition was considered to address the issue of utilizing the network resources and be able to support the network traffic more efficiently.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

We are investigating the impact of more variables taken from quality of service requirements for wireless applications to broaden our multi variable optimization problem. We are still looking into dynamically assigning multiple controllers to the network to be able to back up the system in case of failure as well as secure the communications between the switches and the controller. We are still investigating techniques that allow us to virtualize the controller in the network to avoid a single point of failure due to a hardware/software failure or a network attack.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

This was a great opportunity for the PI to work with Dr. Kandah. This has opened up other opportunities that they can work together on Smart City projects with the goal of securing federal findings. This also opened up opportunities for collaborating with other universities.

This project was a great help for the Co-PI in learning different techniques in traffic engineering and how software can be used to manage the traffic in the network more efficiently. The Co-PI will continue his work in this field and investigate new techniques to help advancing his research capacity and apply the concept to different fields in computer networks such as Internet of Things and Connected vehicles.

Students Impacted

One post-doctoral fellow and three students worked on this project:

- Dr. Khashayar Kotobi is a post-doctoral research fellow under supervision of PI. During the time on this project Dr. Kotobi learn about new research in wireless communication networks and blockchain technology.
- Steven Schmitt perusing his graduate studies in Computer Science. Mr. Schmitt is anticipated to graduate late 2018. Mr. Schmitt focused his research on Software Defined Network and he worked on building the SDN testbed to be used as a platform to test our future research in this field.
- Dylan Brownell and Peyton Ball worked on this project and they are currently perusing undergraduate degree in Computer Science. During the time on this project, Mr. Brownell and Mr. Ball learn a great amount about programming and networking that will serve them well after graduation.

Community and Broader Impacts

Our research will help us gain a better insight into wireless 3C technologies and the fundamental infrastructure to support S&CCs. Also, it has a great potential to transform Chattanooga from Gig City to Wireless Gig City, and eventually to a truly smart and connected city.

Work products reduced to practice; provide a bibliographical entry where appropriate

1. Steven Schmitt and Farah Kandah, "Denial of Service Attacks Prevention using Traffic Pattern Recognition over Software-Defined Network", EAI Endorsed Transactions - Journal: Ambient Systems
2. Farah Kandah and Steven Schmitt, "SAND: Smart and Adaptable Networking Design Using Virtual Slicing over Software-Defined Network", EAI Endorsed Transactions - Journal: Internet of Things
3. Khashayar Kotobi and Mina Sartipi, "Efficient and Secure Communications in Smart Cities using Edge, Caching, and Blockchain", IEEE Smart Cities Conference (ISC2 2018)

Outreach & Collaboration

We collaborated with several academic institutions such as University of Texas Dallas and Auburn University. We also worked very closely with the City of Chattanooga.

EXTERNAL FUNDING

Proposal Submissions

1. NSF S&CC: CI-New: Collaborative Research: A Sandbox for Fostering Smart City Development
2. NSF SaTC: CORE: Small: RUI: vMAP - Mapping Autonomous Vehicle Authentication/Trust Building in Real-time over a Dynamic Adaptive Network
3. NSF CPS: Medium: Collaborative Research: Identity, Trust, and Resilient Architecture for IoT/CPS at Scale

Contracts / Awards Received

None

Sponsored Program Capacity Building Activities

None

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

Our next step in this research is to investigate different techniques in Software-defined networking field that allow us to enhance the network performance in handling traffic smartly as well as investigating the possibility to bring the SDN to communicate and utilize the traffic wirelessly.

We need to study the multi variable optimization problem regarding the quality of service for more variable and evaluate the impact of the overhead caused by this algorithm on data traffic.

We need to investigate the blockchain security protocol and its security strength in terms of DoS and other common attacks. We need to evaluate the power and delay consumptions of miners (nodes that are part of security providers).

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

We will focus our future research to create robust automobile and aerial vehicle networks through the development of cybersecurity layers that can advance the next generation cyber-workforce in standing against threats that target the safety of human lives.

While working on enhancing the wireless network performance for users, we faced the security issue that would arise due to lack of scalability in current security protocols. As a result, we researched blockchain distributed data base as a feasible solution for these security concerns.

What barriers (if any) do you face to reach these next goals?

Seeking more funds to support our future research and train new students to conduct research and use our developed systems.

We need more funds to be able to train new students for security and blockchain aspect of this project. We need to implement and scale a blockchain to test our security protocol and its impact on quality of service of the wireless network.

FINANCIAL ACCOUNTING

Total Award Amount: $92,000.00

Cumulative Expenditures: $79,407.00

Remaining Award Amount: $12,592.00

Supplemental Award Request: $12,592.00

Dr. Kidambi Sreenivas, Lead PI

Co-PI(s): Dr. Abdollah (Abi) Arabshahi
Other Personnel:
David Collao, PhD (*Senior personnel*)
Jhiin Joo (*Graduate student*)

Project Title: "Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications"

Date Submitted: 02/27/2017

Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
Noise from various sources is a part of everyday life. The ability to simulate the generation and propagation of noise is a significant challenge. This is primarily because acoustic waves are a perturbation (very small changes) of the ambient pressure and significant computational resources are required in order to adequately resolve the flow field. The first step in any of these aeroacoustic simulations is to ensure that one has a good representation of the flow physics and that the relevant noise sources are adequately captured. This is accomplished through the use of test cases, data for which has been obtained through experiments.

Discussions with researchers at the NASA Glenn Research Center and the Naval Surface Warfare Center, Carderock Divison results in the identification of two test cases. These were a turbomachinery test case and a flat plate test case. The turbomachinery test case was simulated using Tenasi, while the flat plate test case was simulated using FUNSAFE. The reason for choosing Tenasi for the turbomachinery simulations is that it is a mature code with significantly more capabilities compared to FUNSAFE. Similar capabilities are under development for FUNSAFE.

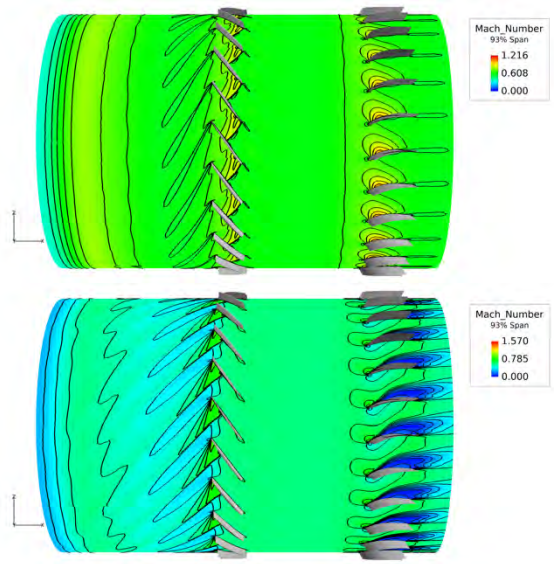
The turbomachinery test case was the SDT2-R4 fan-stage configuration. This particular stage was designed with three different stator configurations: Baseline, Low-vane, and Low-noise. Earlier simulations of the Baseline configuration were carried out using Tenasi and good agreement was obtained with experimental data (for overall performance). In the current project, the low-noise configuration was simulated and excellent agreement was obtained with experimental data (overall performance). These simulations involved meshes that contained 104 million nodes and were run on 224 cores of OneSeventeen at the SimCenter. These simulations provided the baseline validation, which was a necessary first step for the acoustic simulations. The results from these simulations were published in a conference paper at the AIAA Aviation 2018 Conference in Atlanta.

The flat plate test case is being simulated using FUNSAFE. In order to obtain the correct pressure perturbations on the surface of the flat plate, LES (Large-Eddy-Simulation) of the flat plate is being carried out. In order to reduce the computational requirements, these simulations used an approach called rescale-and-reintroduce. This had a significant learning curve associated with it and therefore successful simulations were not obtained within the project time period.

Project Web Page(s):
None

Development of Computational Aeroacoustics Capability for Aerospace/Defense Applications

Technology Area of Interest: Aerospace & Defense

PROPOSED TECHNICAL APPROACH	OPERATIONAL CAPABILITY PROVIDED
The primary goal of the research is to accurately and efficiently compute the unsteady flowfield around geometries of interest with an aim of using that information to compute acoustic information • Task 1: Identify test cases that are of practical importance to the aeroacoustics community • Task 2: Build meshes for cases of interest • Task 3: Apply Tenasi to simulate the identified test cases • Task 4: Apply FUNSAFE to simulate the identified test cases	Noise from various sources is a part of everyday life. The ability to simulate the generation and propagation of noise is a significant challenge. This is primarily because acoustic waves are a perturbation (very small changes) of the ambient pressure. Consequently, significant computational resources are needed in order to resolve these waves accurately. A recent advance in high-order algorithms enables one to increase the order of accuracy (instead of or in addition to increasing spatial resolution) locally. This could have significant implications for acoustic wave propagation as it could drive down the cost of these simulations. The proposed research will focus on applying high-order techniques to canonical and practical problems in aeroacoustics.
RESULTS	**OTHER INFO**
 Figure 1: Geometry and flow solution for the Low-Noise configuration of the SDT2-R4 test case	**Budget and Schedule** Total Budget: $68,085.00 Actual Used: $68,085.00 Balance: $ 7,505.03 Total period of performance is 12 months. Task 1: Months 1-4 Task 2: Months 3-6 Task 3: Months 5-12 Task 4: Months 5-12 **Deliverables** • Monthly Technical Report: Describing numerical methods, techniques and results that were developed or improved. • Progress/Status Report: Final Report **Organization Information** UTC-SimCenter, Dr. Kidambi Sreenivas 701 East M.L. King Boulevard, Chattanooga, TN 37403 Telephone: 423-425-5506 Email: Kidambi-Sreenivas@utc.edu

Project Overview

Computational Simulations of the Low-Noise SDT2-R4 Configuration Using *Tenasi*

Kidambi Sreenivas[1], Robert S. Webster[2], and M. David Collao[3]
The University of Tennessee at Chattanooga, Chattanooga, TN, 37403

The SDT2-R4 fan-stage, the focus of this study, has been used for aeroacoustic testing at NASA Glenn. As part of the aeroacoustic testing, performance data on the fan and the fan-stage were obtained. The fan-stage had three stator vane configurations. Earlier computations carried out by the authors had focused on the baseline stator vane configuration consisting of 54 vanes. The current study focuses on the performance prediction of the low-noise configuration which consists of 26 swept vanes. In an effort to reduce computational cost and assess its impact on performance prediction, two axisymmetric configurations were considered. The first was a 1/22nd wheel (required blade count modifications) and the second was a half-wheel configuration. Good agreement was obtained between the computations and experimental data, though there was a slight over-prediction of adiabatic efficiency for both configurations.

I. Introduction

COMPUTATIONAL simulations of axial-flow compressors started to come into their own in the early to mid-1990's, and there have been many publications of such simulations on single-stage machines. Due to limitations in computational capabilities (e.g., memory capacity, the use of only one processor, etc.), simulations of multistage machines were, by and large, simply not practical. Significant increases in computing capacity, both in terms of memory and processor speed, as well as parallel processor machines and flow solvers, have made the ability to run large jobs relatively routine. As such, the ability to conduct multistage turbomachinery simulations has been around for a number of years now. An early example is given in a summary article by Adamczyk**Error! Reference source not found.** in which simulations of a 4-stage low-speed research compressor and a 10-stage high speed compressor, among others, were simulated using the average-passage methodology. This same methodology was used as far back as the late 1980's by Adamczyk et al.**Error! Reference source not found.** for simulating a one-and-a-half stage turbine. Gopinath et al.**Error! Reference source not found.** implemented an extension to the harmonic balance method and used it to simulate the NASA Stage 35 compressor, as well as the middle three rows (stator-rotor-stator) of a 5-row, two-dimensional compressor geometry**Error! Reference source not found.**. Van Zante et al.**Error! Reference source not found.** used the MSU-TURBO solver to simulate a 2-1/2 stage, high-speed compressor. This involved a large-scale simulation that compared the computational cost of a full-wheel simulation to one using the phase-lag boundary condition. These are but a few examples of past computational efforts on multistage machines.

Increases in the availability of computational resources have lead to improvements in performance predictions for single and multi-stage machines. With these improvements, the ability to predict noise from high- and ultra-high bypass engines is improving. A series of tests were carried out at NASA Glenn utilizing the so-called SDT2-R4 rotor that included aerodynamic (performance) as well as aeroacoustic measurements. This data set has served as the test case for the fan broadband noise prediction workshop**Error! Reference source not found.** held as part of the 22nd AIAA/CEAS Aeroacoustics Conference in France (2016). A necessary first step towards computing broadband noise is the ability to predict the performance of the fan stage. This is particularly true for the cases where the fan tip speed is supersonic.

The machine of interest for this paper is a single stage axial-flow fan (the aforementioned SDT2-R4 fan stage) that is a scaled version of a relatively modern turbofan. This machine was tested using the same rotor, but with three different stator configurations, i.e., Baseline, Low Count, and Low Noise. The baseline configuration has been

[1] Associate Professor, Department of Mechanical Engineering and SimCenter; AIAA Senior Member.
[2] Associate Professor, Department of Mechanical Engineering and SimCenter; AIAA Senior Member.
[3] Research Associate, SimCenter

One of the primary challenges in performing a computational simulation of a rotating machine, whether a pumping device or a turbine, is due to the fact that these are often large-scale efforts involving meshes with millions of points and the more rows of the machine that are involved, the larger the computational demands. As long as the simulations are in the stable portion of the machine's operating region, a suitable approximation can often be made by simulating a relatively small sector of the wheel. However, this will oftentimes require that compromises be made in the number of rotor blades and/or stator vanes that are actually included in the simulation. In the results presented here, two sets of simulations are conducted. The first involves a $1/22^{nd}$-wheel simulation, which involved a change in the number of stator vanes (compared to the experiment) that were included in the simulation. The second involves a half-wheel simulation which had the correct number of rotor blades and stator vanes as compared to the experiment.

The remainder of the paper is laid out as follows: Highlights of the various features of *Tenasi* will be given in the sections II. Section III provides a description of the geometry and the modifications that were made. Section IV will contain the bulk of the material, as it will be a presentation and discussion of the results. Finally, conclusions will be presented in section V.

I. Flow Solver

The baseline flow solver in *Tenasi* employs a finite volume, implicit scheme with high resolution fluxes and a dual time stepping, Newton sub-iteration procedure for time accuracy. The linear system at each time step is solved using a Symmetric Gauss-Seidel algorithm. Some of the features of the unstructured solver are highlighted below. The details of the numerical algorithm are available in Hyams et al.**Error! Reference source not found.**

A. Flow Regimes

An important distinguishing feature of *Tenasi* is that the same executable can be used to solve different sets of governing equations, i.e., iso-energetic incompressible**Error! Reference source not found.**, incompressible with heat transfer**Error! Reference source not found.**, compressible, preconditioned compressible**Error! Reference source not found.**, surface capturing, electromagnetics, etc. by choosing a flow regime at runtime. The implementation is such that a new flow regime can be added in a fairly straightforward manner by implementing the required flux functions and the boundary conditions. The rest of the infrastructure such as processing of the grid, the sliding interface capabilities, the solution of the linear systems etc. are available to all flow regimes. For the present study, preconditioned compressible formulation is utilized. However, given the higher Mach numbers present in the domain, preconditioning is disabled and the solver utilizes a primitive-variable formulation.

B. Residual Computation

The unstructured solver is based on a node-centered formulation. Higher order spatial accuracy is achieved using a linear or quadratic reconstruction of the dependent variables at the control volume faces and using these reconstructed values to evaluate the fluxes. Viscous terms are evaluated using a directional derivative based approach. The gradients required for the variable reconstruction are computed using an un-weighted least squares approach while the gradients for the viscous terms are computed using a weighted least squares approach. The numerical fluxes are evaluated using either Roe's flux difference split approach or an HLLC approach. In this particular case, the HLLC fluxes are used.

C. Time Evolution

The flow solver employs a discrete Newton relaxation approach coupled with dual time-stepping to solve the unsteady equations. The dual time stepping approach is used to accelerate the convergence of the unsteady residual. Newton's method is used to drive the unsteady residual to zero, thereby ensuring time accuracy. The flux Jacobians arising from this linearization can be evaluated using numerical derivatives or the complex Taylor series method. They can also be replaced by approximations which result in substantial savings in computational time. The resulting linear system is solved using a Symmetric Gauss Seidel algorithm (point relaxation). For deforming grids, the Geometric Conservation Law (GCL) has to be satisfied in order to prevent the occurrence of spurious sources in the solutions. This leads to an additional contribution to the residual.

D. Turbulence Modeling

The turbulence models are implemented in a loosely coupled manner. The flow solver has the Spalart-Allmaras model, the Menter SAS model, the k-ε/k-ω hybrid model (with and without SST), the standard k-ε model, the Wilcox k-ω model, and the Wilcox Reynolds Stress model. In addition, DES modes are available for the Spalart-Allmaras, the Menter SAS and the k-ε/k-ω hybrid models. Furthermore, a wall adapting LES model (WALE) is also available.

A. Parallel Implementation

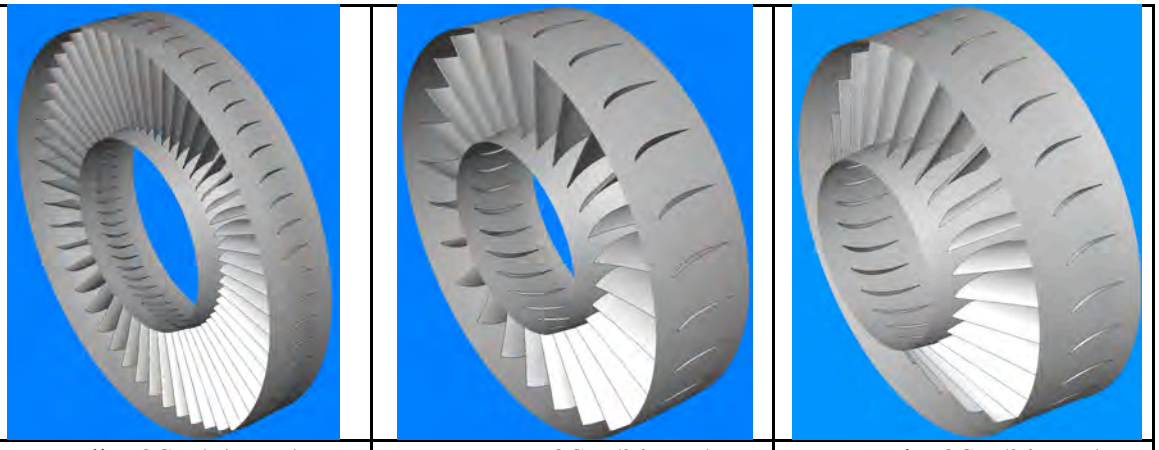
The parallel solution procedure consists of a scalable solution algorithm implemented to run efficiently on subdomains distributed across multiple processes and communicating through MPI. The algorithm has multiple nested kernels viz. time step, Newton iteration, LU/SGS iteration etc., and the subdomain coupling is at the innermost level, i.e., in the solution of the linear system. A block-Jacobi type updating of the subdomain boundaries ensures efficient parallelization with a small incremental cost incurred in terms of sub-iterations required to recover the convergence rate of the sequential algorithm. Details about the parallel algorithm can be found in Hyams.**Error! Reference source not found.**

B. Relative Motion

The unstructured sliding interface technique utilized in *Tenasi* was developed and validated at UTC. The underlying concept is to extrude the pairs of sliding interfaces into adjoining domains and to interpolate for the flow variables and their gradients at the newly created nodes. Note that the sliding interfaces are not merged in any way and this has the potential to lead to multi-valued solutions at a given point. However, this has not been observed in practice and points that are very close to each other have approximately the same solution values. Further details on the parallel implementation of the sliding interface algorithm are available in Hyams et al.**Error! Reference source not found.**

I. Problem Description and Setup

The SDT2-R4 turbofan stage, which is a 1/5 scale model simulator representing the bypass stage of a 2002-era high bypass ratio turbofan engine, has been used in baseline aeroacoustic testing at the NASA-Glenn 9x15 Low Speed Wind Tunnel. The test configuration consisted of the bypass fan and outlet guide vanes in a flight-type nacelle, with three different OGV configurations (Figure 1). The rotor was the same for all three configurations and all simulations have been carried out at a nominal corrected design speed of 12,657 RPM. The tip diameter of the rotor blades is 22 inches, giving a design tip speed of 1,215 ft/s and a tip Mach number of approximately 1.09. At the design point, the corrected mass flowrate is 100.5 lbm/s. Based on the description of the geometry, a small tip gap region is included between the rotor tip and casing to allow for tip-gap leakage flow.



Baseline OGV (54 vanes)	Low-count OGV (26 vanes)	Low-noise OGV (26 vanes)

Figure 1: The various OGV configurations available for the SDT2-R4 fan stage

In earlier work**Error! Reference source not found.**,**Error! Reference source not found.**, the baseline OGV's were utilized; thus, the stage consisted of 22 rotor blades and 54 stator vanes. The actual simulations of the baseline OGV's were carried out on a $1/11^{th}$ sector with axisymmetric boundary conditions. The axisymmetric simulation requires the addition of one vane in the stator section so that a whole number of blades/vanes can be simulated (for a 22-55 stage). While this is not a drastic change to the original geometry, the solidity ratio is increased slightly; as such, it is expected that a slightly lower overall mass flowrate will be allowed through the stage than in the experimental tests, which use a 22-54 stage. It should be noted, however, that this variation in solidity is, on average, the same as the variation in solidity between the baseline, low-noise, and low-count OGV's used in Hughes.**Error! Reference source not found.**

baseline OGV; therefore, the losses are expected to be greater. The reason for the aft sweep was to reduce the tone noise by increasing the axial spacing between the fan and the OGV, resulting in a weakening of the acoustic wave from the fans by the time it strikes the vanes. Additionally, the sweep of the vanes ensures that the fan wake does not strike the leading edge of the OGV all at once, but rather intersects the swept vane leading edge in a scissor-like fashion resulting in an overall reduction in the noise generated. The focus of this paper is on the aerodynamic performance of the SDT2-R4 fan stage with the low-noise OGVs.

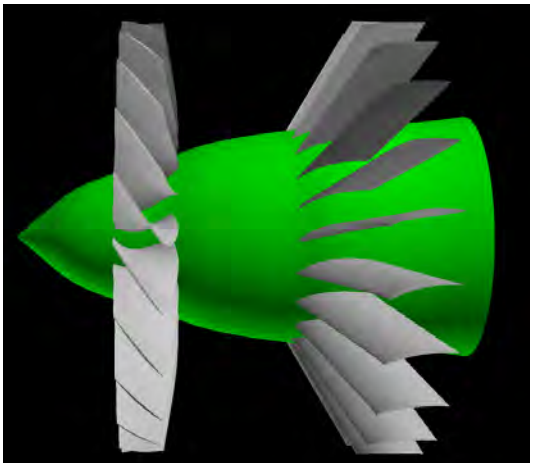


Figure 1: Geometry of the SDT2-R4 fan stage with the low-noise OGVs (casing not shown)

The minimum sector size that could be achieved without modifying the blade counts was 180°, which would result in a simulation consisting of 11 rotor blades and 13 stator vanes. In order to reduce the computational requirements, 4 vanes were removed from the OGVs, thereby allowing a 1/22nd sector to be simulated. This is a significant change compared to the earlier simulations and its impact on the predicted performance could be significant. The changes in the blade counts are summarized in Table 1, with numbers in red indicating changed counts. In the results presented here, aerodynamic performance of the fan-stage using the half-wheel as well as the 1/22nd sector are compared to each other as well as experimental data.

Table 1: Blade/vane counts for half-wheel and 1/22nd sector simulations

Blade/Vane Row	Rotor	Stator	% change (Rotor)	% change (Stator)
Original Counts	22	26	N/A	N/A
Half-Wheel Counts	11	13	0	0
1/22nd Sector Counts	1	1	0	-15.39%

I. Results and Discussion

A. Simulation of the 1/22nd-wheel configuration

Given the similarity between the two sets of simulations, the majority of the description regarding the actual running of the simulations will be concentrated in this section. The grid is unstructured in nature, and it contains a combination of quadrilateral and triangular surface elements and hexagonal, pyramidal, prismatic, and tetrahedral volumetric elements. **Error! Reference source not found.** summarizes the approximate counts of the respective surface (triangles, quadrilaterals) and volume (tetrahedra, pyramids, and prisms) elements, as well as the total node count for the 1/22nd-wheel configuration. The overall domain was then divided into 48 sub-domains to run on the in-house parallel cluster. Typical runtimes were on the order of a few hours for the near-choke points while it increased to about a 1.5 days for the near-stall points.

The simulations were started in a steady-state mode with the CFL being ramped up from 1.0 to 5.0 over 360 time steps. The steady-state simulation was carried out for a total of 1800 time steps with the first 360 being first order in space. The simulation was then restarted in a time-accurate mode and was run for a further 1800 steps. The time step used for the simulations corresponded to 360 per revolution and the time-accurate simulations utilized 4 Newton

sub-iterations to ensure time accuracy. A dual-time-stepping approach was used to improve the robustness of the unsteady simulations. All results presented here were obtained using a one-equation SAS turbulence model and the governing equations were solved in a primitive variable form with density, velocity and pressure as the independent variables. Simulations were stopped when the mass flow rates between the exit and the inlet were within 0.25%. The simulations for the higher back pressures (lower mass flow rates) were restarted from the previous stable operating point in order to reduce the computational time to solution.

Table 1: Summary of mesh characteristics for the 1/22nd-wheel configuration

Surface/Volume/Node Elements/Points	Triangles	Quads	Tets	Pyramids	Prisms	Hexahedra	Node Points
Approximate Counts in Millions	0.91	0.058	21.8	0.11	12.23	0.001	10.03

Results are presented here for the fan-only and the stage performance. The fan-only results were obtained by evaluating the performance parameters for the fan even though it was part of the stage simulation. This was done in order to mimic the experimental approach wherein the fan only performance was derived from measurements taken for the entire stage.

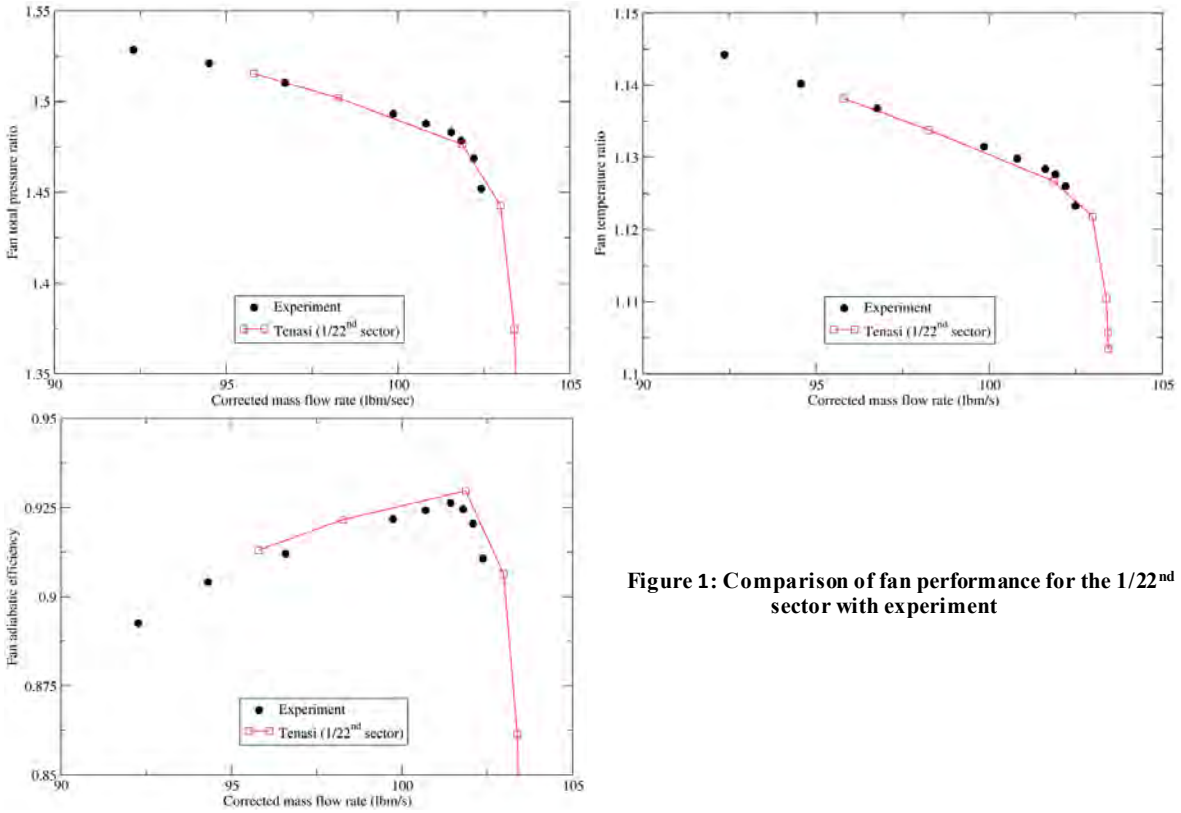


Figure 1: Comparison of fan performance for the 1/22nd sector with experiment

Figure 1 shows a comparison of the fan performance. As can be seen from the figure, very good agreement is obtained between the computations and experiment for the total pressure and temperature ratios. Adiabatic efficiency is over predicted a little, but the overall agreement is still good. The simulations were not extended to the lower mass flow rates because numerical stall was encountered. The possible reasons for this are detailed in a later section where the relative performance of the 1/22nd- and half-wheel configurations are discussed. **Error! Reference source not found.** shows the computed performance of the stage compared to the experiment. Again, good agreement in the total pressure ratio is obtained, while the predicted efficiency is higher than the experiment. The close agreement obtained for the fan-only results indicates that the loss mechanisms are not being sufficiently captured in the stator vanes. This leads to an under prediction of the enthalpy rise in the stage, which consequently results in an over prediction of the adiabatic efficiency.

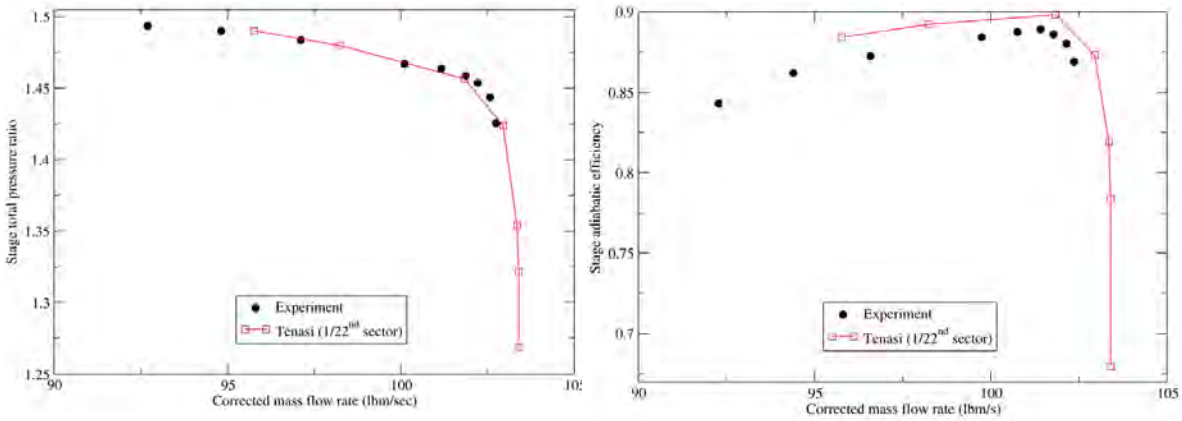


Figure 1: Comparison of stage performance with experiment for 1/22nd sector simulations

A. Simulation of the half-wheel configuration

This simulation was significantly larger than the 1/22nd-wheel configuration. As can be seen from Table 1, the mesh here consisted of 104.4 M nodes and was partitioned into 224 subdomains. Again, the simulations followed the same procedure described for the 1/22nd-wheel configuration. The only differences were in the number of time steps employed per revolution. As the simulation approached the numerical stall point, the number of time steps per revolution was increased from 360 to 900. This was to enable capturing of any unsteadiness that could arise as one approached the numerical stall point. These simulations required approximately 60 seconds per time-step in the unsteady mode. Typical simulations required about a week of runtime, with the near-stall points requiring on the order of two weeks of runtime.

Table 1: Summary of mesh size for the half-wheel configuration

Surface/Volume/Node Elements/Points	Triangles	Quads	Tets	Pyramids	Prisms	Node Points
Approximate Count in Millions	8.39	0.27	181	1.22	143.4	104.4

Results for the half-wheel configuration are presented in a manner similar to the 1/22nd-wheel configuration. **Error! Reference source not found.** shows the comparison of the fan-only performance, while **Error! Reference source not found.** shows the same for the stage. The trends for these two figures follow very closely the ones observed for the 1/22nd-wheel configuration. The total pressure and temperature rise is captured quite accurately, though the temperature ratio is under predicted (for both the fan and the stage). This is indicative of the not having enough loss in both the rotor as well as the stage. The consequnce of this is that the adiabatic efficiency is higher than the experimental values for both the fan-only as well as the stage. The losses for the stage computations are not as high as the experiment as evidenced from the over prediction of the adiabatic efficiency. Furthermore, the losses in the rotor The biggest difference between the two sets of simulations is that stable operating points were obtained for the half-wheel simulations well beyond the numerical stall point for the 1/22nd-wheel simulations.

B. Comparison of 1/22nd- and half-wheel simulations

Error! Reference source not found. compares the predicted performance between the 1/22nd wheel and the half-wheel simulations. As can be seen from the table, the comparison between the various parameters is very close between the two sets of simulations. The biggest differences arise as one nears the numerical stall point (defined as when the code starts producing NaN's). The last stable operating point obtained for the 1/22nd wheel is a back pressure of 127.5 kPa, while the half-wheel simulation is stable up to a back pressure of 130.75 kPa. This behavior is a little unexpected as the solidity of the stator vane-row was reduced for the 1/22nd wheel case (recall that 4 vanes were removed in order to create the 1/22nd wheel geometry) compared to the half-wheel case. A possible reason for this could be that the removal of the vanes causes the gap between the vanes to increase, which in turn leads to reduced acceleration between the vanes. Furthermore, the increase in the vane pitch leads to the suction side of one vane not "feeling" the pressure side of a neighboring vane. Therefore, even though there is a decrease in the solidity of the

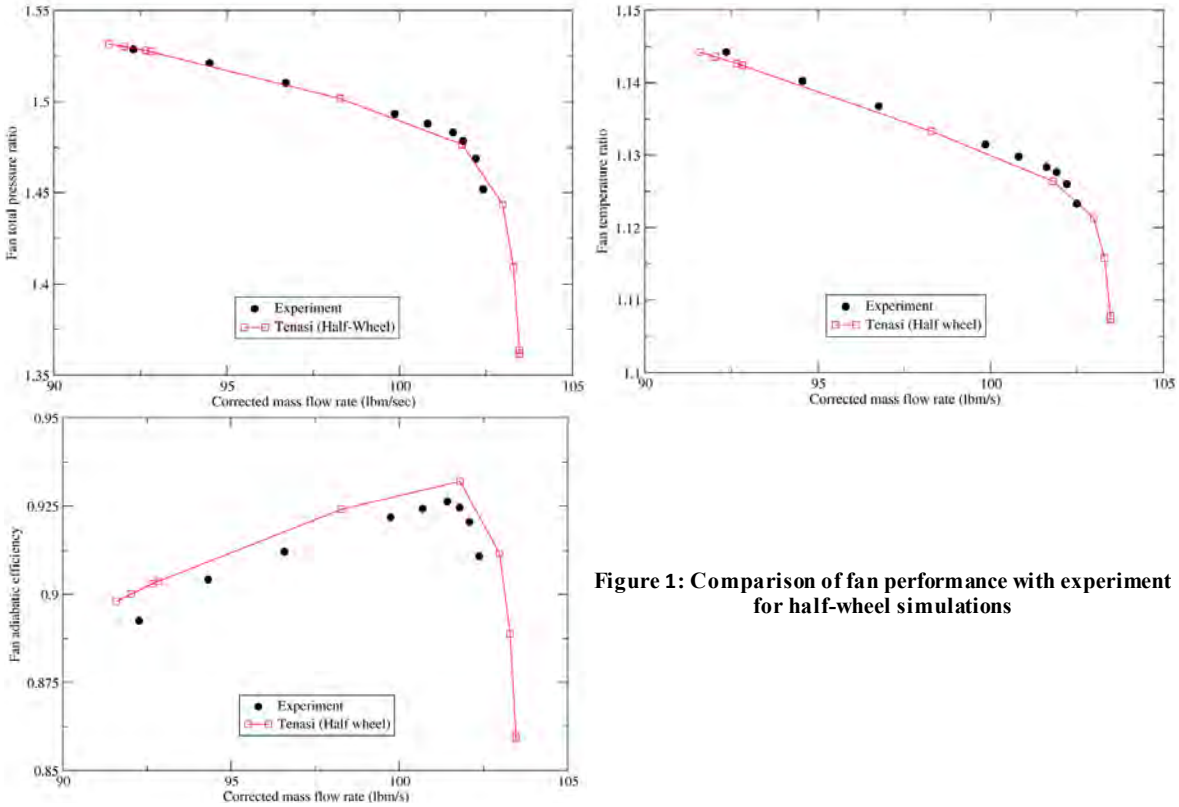


Figure 1: Comparison of fan performance with experiment for half-wheel simulations

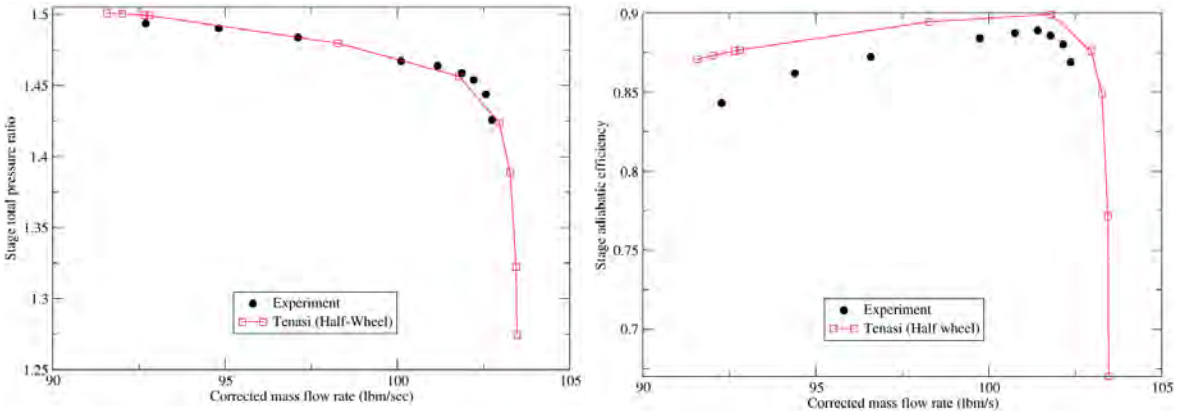


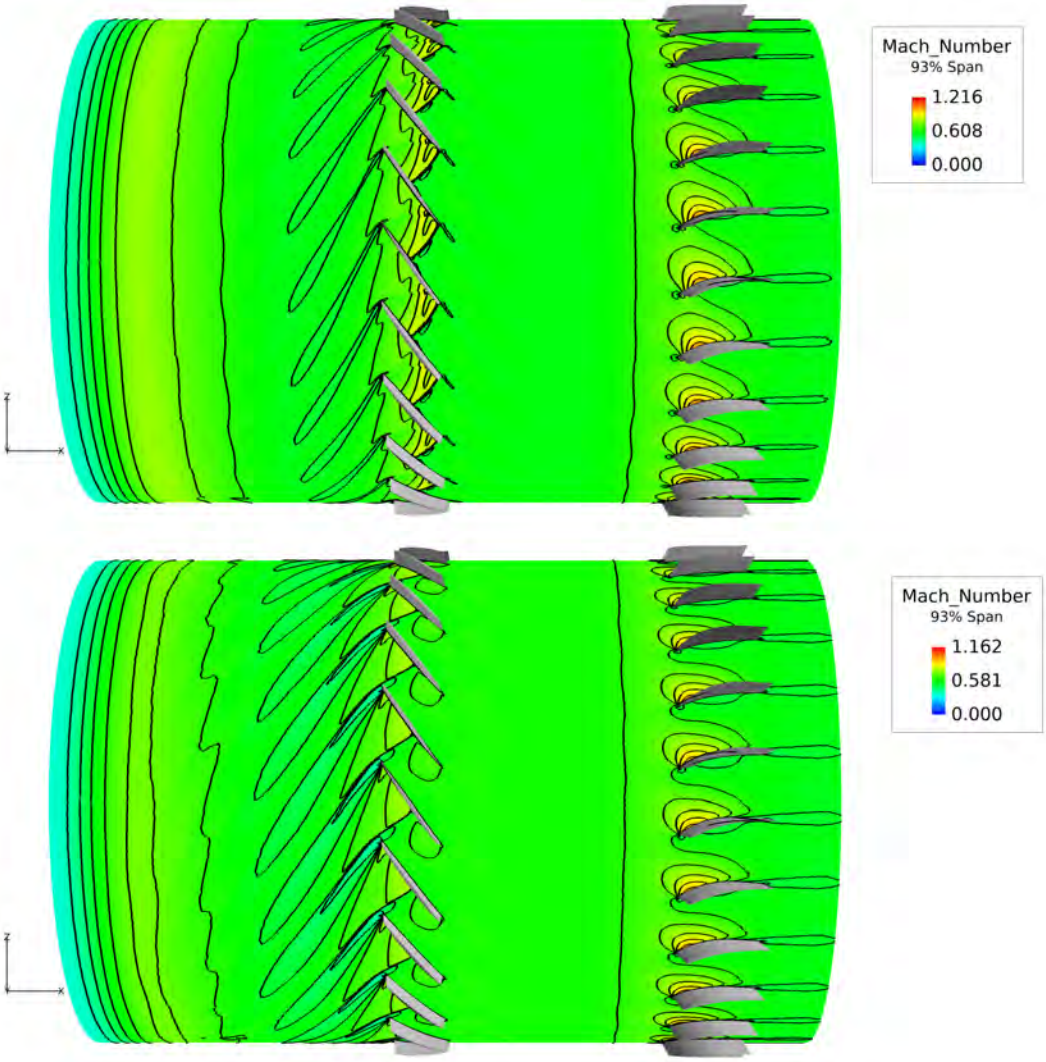
Figure 2: Comparison of stage performance with experiment for half-wheel simulations

Table 1: Comparison of predicted stage performance between 1/22nd and half-wheel simulations

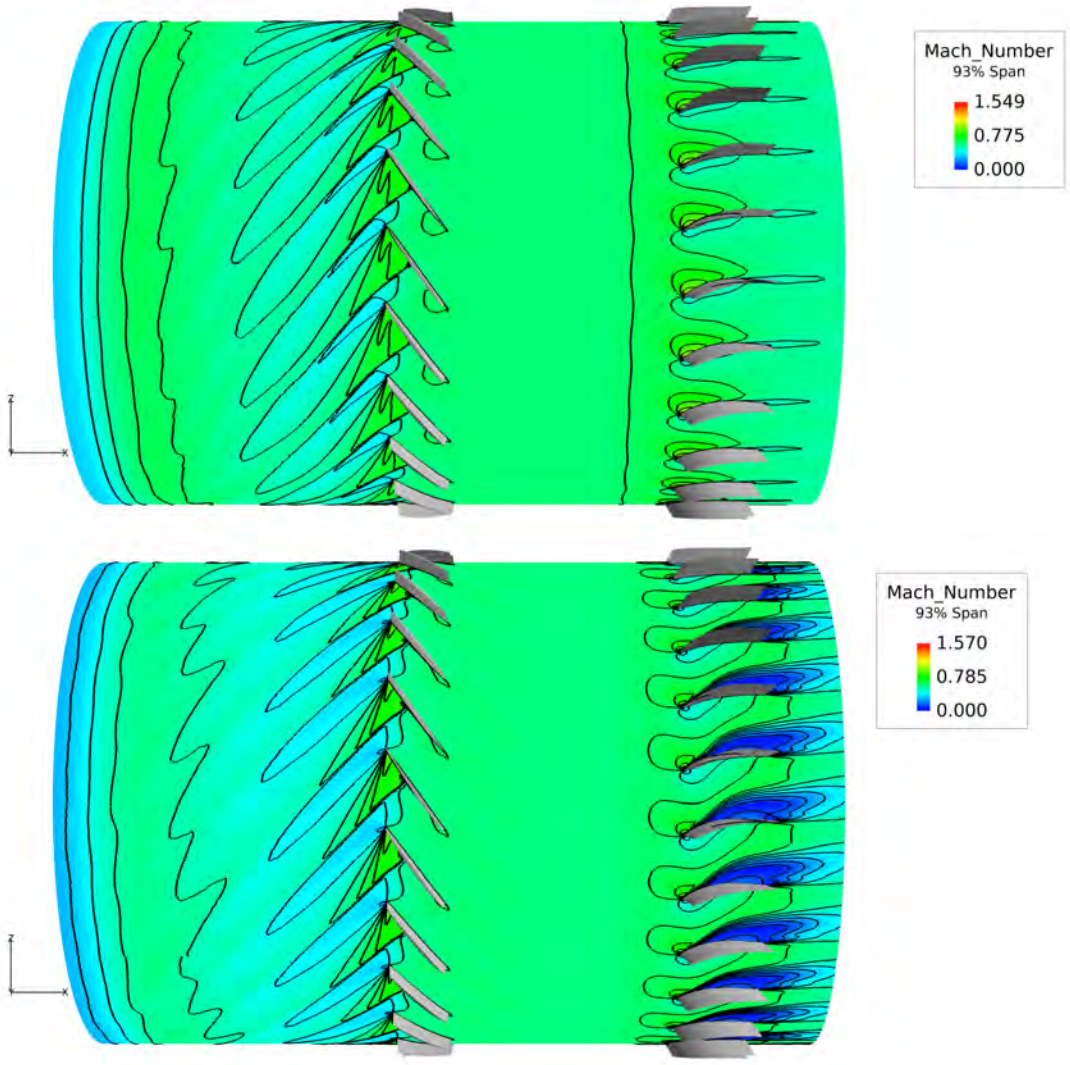
Back Pressure (kPa)	Mass flow rate (kg/s)		Pressure ratio		Temperature ratio		Adiabatic Efficiency	
	1/22nd	Half	1/22nd	Half	1/22nd	Half	1/22nd	Half
90.0	46.902	46.93	1.269	1.275	1.103	1.107	0.679	0.670
100.0	46.899	46.92	1.321	1.322	1.106	1.108	0.784	0.771
115.0	46.697	46.701	1.424	1.424	1.122	1.121	0.873	0.876
120	46.191	46.171	1.457	1.456	1.126	1.126	0.898	0.899
125	44.559	44.575	1.480	1.480	1.133	1.132	0.892	0.895
127.5	43.441	N/A	1.490	N/A	1.137	N/A	0.842	N/A
130.0	Numerical Stall	42.097	Numerical Stall	1.499	Numerical Stall	1.140	Numerical Stall	0.877
130.75	Numerical Stall	41.53	Numerical Stall	1.501	Numerical Stall	1.141	Numerical Stall	0.871
131.0	Numerical Stall	Numerical Stall	Numerical Stall	Numerical Stall	Numerical Stall	Numerical Stall	Numerical Stall	Numerical Stall

A. Flow visualization for the half-wheel case

Figures 7 – 10 show contours of Mach number at 93% span for near choke, peak efficiency, near stall, and stall cases respectively. They correspond to back pressure (from Table 4) of 100 kPa (near choke), 125 kPa (peak efficiency), 130 kPa (near stall) and 131 kPa (numerical stall). At the low back pressure case (Figure 7), the shocks in the rotor are well within the passage, and the stator flow is completely attached. As the backpressure increases (Figure 8), the shock in the rotor passage moves upstream to the point where it is coming off the leading edge of the rotor blade and impacting the adjacent blade about mid-chord.



As the backpressure increases further (Figure 9), the shock in the rotor blade passage is now upstream of the leading edge and the stator vanes are beginning to exhibit a little bit of flow separation. Once the back pressure increases beyond this point, the shock in the rotor blade row moves further upstream. The dramatic changes though occur in the stator vanes. The flow there is completely separated and the increase in blockage results in a significant drop-off in the mass flow rate. Continuing the simulation beyond this point leads to a continual decrease in the mass flow rate and eventually, the simulation crashes, indicating that numerical stall has been achieved.



I. Conclusions

Good agreement was obtained between the computations and experiment for both the 1/22nd- and half-wheel configurations. Both sets of computations over predicted the adiabatic efficiency, which is indicative of under predicting the losses. The half-wheel configuration was able to obtain stable operating points well beyond those obtained using the 1/22nd-wheel configuration. A possible explanation of this behavior arises from the fact that the increased pitch in the stator vane row is limiting the favorable pressure gradient, thereby increasing the propensity to stall. It can also be concluded from these computations that operating points away from the stall point can be computed efficiently using the 1/22nd-wheel configuration. This results in significant computational savings over the bulk of the operating envelope.

Acknowledgments

The authors would like to thank the Tennessee Higher Education Commission through a CEACSE award for the support of this work. Computing resources were provided by the SimCenter at the University of Tennessee at Chattanooga, through a grant from the UC Foundation. Images were created by using FieldView as provided by Intelligent Light through its University Partners Program.

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List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Identify test cases that are of practical importance to the aeroacoustics community	The PI attended an acoustics working group meeting held at NASA Glenn and the AIAA Aeroacoustics conference (co-located with the AIAA Aviation 2017) in Denver. Following discussions with various researchers, the SDT2-R4 and the flat plate case were identified as potential test cases.
Apply Tenasi to simulate the identified test cases	Tenasi was used to obtain the overall performance of the low-noise configuration of the SDT2-R4 test case. Excellent agreement was obtained with experimental data.
Apply FUNSAFE to simulate the identified test cases	FUNSAFE was used to simulate the flat plate test case. These simulations are ongoing and no satisfactory results were obtained within the project time period.

Challenges & Strategies Used to Address / Overcome:

One of the biggest challenges faced during this project time frame was the availability of qualified grid generation personnel. This problem was somewhat mitigated when we had David Collao help us when he could. However, this is not a long term solution and in order to provide one such solution, we have taken to training undergraduate students in the process of grid generation. At the current point in time, we have about 5 students who are capable of generating meshes. They need to continue their training so that they are capable of generating meshes on complex configurations.

The other challenge that is ongoing is the ability to simulate LES type flows using FUNSAFE. This is not a limitation of the software per se, but our lack of experience with such flows and the rescale-reintroduce technique. We've been working with researchers at the Naval Surface Warfare Center, Carderock Division and others who have done this in the past, and are hopeful of improved results.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

The rescale/reintroduce method for the LES simulations did not work as expected. This is an ongoing problem and as mentioned earlier, we're working with various researchers (who have experience with this) in order to get it solved. While the performance of the various configurations were simulated accurately with Tenasi, work is ongoing in order to simulate the acoustics. This will require significantly larger meshes. Currently, the porting of FUNSAFE to use GPU architectures is being pursued. Once that is completed, we can use the improved accuracy resulting from the stabilized finite-element approach in order to reduce the mesh size. This should make the problem more tractable.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

Closer working relationship with NASA Glenn and Naval Surface Warfare Center, Carderrock Division.

Students Impacted

Jhiin Joo, PhD candidate

David Collao, Research Associate, SimCenter

Hannah Gifford, Undergraduate, Mechanical Engineering

Juan Hernandez, Undergraduate, Mechanical Engineering

Community and Broader Impacts

N/A

Work products reduced to practice; provide a bibliographical entry where appropriate

Non-refereed conference:

1. Kidambi Sreenivas, Robert Webster, and Max D. Collao. "Computational Simulations of the Low-Noise SDT2-R4 Configuration Using Tenasi", 2018 Applied Aerodynamics Conference, AIAA AVIATION Forum, (AIAA 2018-4203)

Presentations:

1. Kidambi Sreenivas, “Computational Simulations of Low-Noise SDT2-R4 Configuration Using Tenasi,” AIAA Aviation Forum, Atlanta, GA, June 2018.
2. Kidambi Sreenivas, “Computational Simulations of Rotating Machinery,” NASA Glenn Research Center, October 2017.

Outreach & Collaboration

Visited Mark Celestina and Tim Beach at the NASA Glenn Research Center, Cleveland, OH.

Attended the NASA Acoustics Technical Working Group Meeting at NASA Glenn

EXTERNAL FUNDING

Proposal Submissions

None (as of now). We’re keeping an eye on any upcoming opportunities that are related to the research pursued here and will submit proposals as required.

Contracts / Awards Received

NDA agreement with SmartTruck Inc. for analysis of flows past Class 8 trucks.

Sponsored Program Capacity Building Activities

Attended the NASA Acoustics Technical Working Group Meeting at NASA Glenn

Attended the AIAA Aeroacoustics Conference held at Denver as part of AIAA Aviation Forum

WHAT’S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

We’re pursuing research into developing high-order accurate algorithms that run efficiently on CPU/GPU hybrid platforms. The high-order accuracy should reduce the mesh requirements and therefore make the acoustics problem more tractable. We’re still working closely with researchers at NASA and NSWCCD, so as we generate improved results, we will engage with them to pursue future funding opportunities.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

The porting of FUNSAFE and Tenasi to ARM platforms in underway. Additionally, FUNSAFE is currently being ported to GPUs, which should enhance its overall capability to solve problems of practical interest. This research is being pursued jointly with Craig Tanis, James Newman, Robert Webster, and Abi Arabshahi. Once the initial porting of FUNSAFE is complete, it will be enhanced to solve problems from various solution domains (and mixed domain problems like fluid-structure, fluid-thermal, fluid-structure-thermal etc.).

What barriers (if any) do you face to reach these next goals?

Time.

FINANCIAL ACCOUNTING

Total Award Amount: $68,085.00

Cumulative Expenditures: $60,582.00

Remaining Award Amount: $7,503.00

Dr. Endong Wang, Lead PI

Co-PI(s): Dr. Neslihan Alp
Other Personnel:
Graduate Student: Raghda Mohamed

Project Title: "Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings"

Date Submitted: 02/27/2017

Award Start - End Date: July 1, 2017 – June 30, 2018

Non-Technical Summary:
Effective energy efficiency upgrading through targeted retrofitting on commercial buildings appears to offer a significant opportunity to the overall success of sustainability strategy in the U.S., due to their material share in the totaled building energy consumption of the nation. Per the most recent report of the U.S. Energy Information Administration (EIA), commercial building energy systems consumed 4.29 quintillion joules of primary energy accounting for more than 38% of those used by stock buildings in the country.

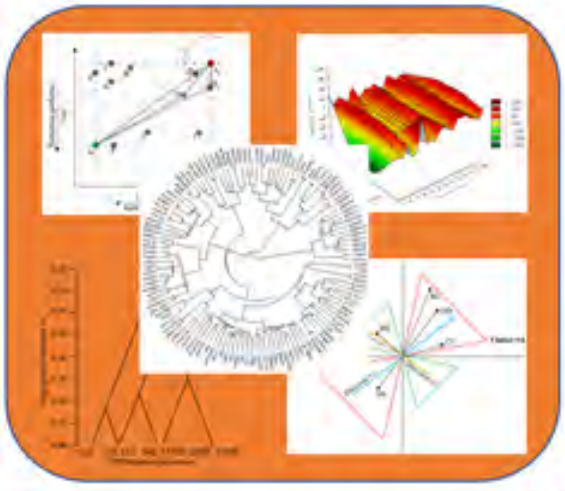
Meanwhile, as an initial departing point, robust fault detection through various diagnosis methods, such as visual inspection, blower door test, infrared thermography and data-driven benchmarking assumes a nontrivial role in a successful energy retrofitting initiative. Minor errors from diagnosis process could result in severe mistakes in discovering energy faults and eventually costly failure of an energy retrofitting investment. Nevertheless, the complicated static and dynamic, physical and non-physical interactions among building structure, envelope materials, heating, ventilating, and air conditioning (HVAC), plumbing systems, climate conditions, as well as occupants' behavior render building energy performance evaluation an uneasy task. The key challenge arises from the dilemma that the pool of energy factors that have been documented to potentially affect energy performance of commercial buildings is extremely large, due to the above complicated concurrent interactions.

Multi-criteria benchmarking is emerging as a more rational option over the traditional single-angle method to assess building performance which is fundamentally of multifactor nature. Nevertheless, existing multifactor performance diagnosis procedures tend to ignore the common issue of multicollinearity trap which could result in misleading decisions. Combining with information theory, this project intends to develop models for building energy performance assessment in a multi-factor manner to facilitate energy retrofitting programs.

Project Web Page(s):
None

Robust Multifactor Framework for Large-scale Fault Detection and Diagnosis in Energy Systems of the U.S. Commercial Buildings

Technology Area of Interest: Energy and Environment

PROPOSED TECHNICAL APPROACH	OPERATIONAL CAPABILITY PROVIDED
This project is to develop a robust multifactor, multi-level instrument for building energy performance evaluation. • Task 1: The proposed analysis framework is established • Task 2: Data are collected • Task 3: The required data collection is completed. The obtained data are preliminarily analyzed • Task 4: The obtained data are formally analyzed. Results/findings are finalized	Though significantly improved, Chattanooga, as one of the "dirtiest" U.S. cities identified by EPA in 1969, still has much space to be healthier and environmentally cleaner through building sustainability programs in view of its large body. Compared to our previous research, this project is more systematic and beneficial with improved implementation capability for energy retrofitting application.
RESULTS	**OTHER INFO**
 Figure 1: Building energy analysis outcomes	**Budget and Schedule** Total Budget: $49,902.00 Actual Used: $46,415.00 Balance: $ 3,487.00 Total period of performance is 12 months. Task 1: Months 1-3 Task 2: Months 4-7 Task 3: Months 8-9 Task 4: Months 10-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work **Organization Information** UTC-Engineering Management Dr. Endong Wang 615 McCallie Ave, Chattanooga, TN 37403 Telephone: 423-425-5778 Email: Endong-Wang@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Aim: This project is to develop a robust multi factor multi level (MFML) instrument for building energy performance evaluation. Compared to our previous research, this project is more systematic and beneficial with improved implementation capability for energy retrofitting application.

Methodologies: Advanced statistical learning and data mining techniques, including variable clustering, principal component analysis and random forest, were used to decompose the verifiable core-factor-structure of building energy performance.

Activities: 1) Develop analysis framework; 2) Collect data through database extraction; 3) Analyze data and summarize findings; 4) Draft papers and proposals; 5) Disseminate research achievements through high-impact journals and conferences, and also integrate them into ENGM 5600 LEED and Sustainability course.

Outcomes: Three high-impact journal papers and three international conference papers have been drafted/submitted/published to disseminate the achievements of the proposed project. Eight internal/external proposals were submitted to UTC, ORAU, NSF, TDOT and NAHB. Five of them were funded.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
The proposed analysis framework is established	Variable clustering based factor analysis framework was developed.
Data are collected	Data on commercial buildings were extracted/collected.
The required data collection is completed. The obtained data are preliminarily analyzed	Data were preliminarily processed and verified to be valid.
The obtained data are formally analyzed. Results and findings are finalized	Data were formally analyzed using the developed framework.
Papers are drafted	Papers were drafted/submitted/published.

Challenges & Strategies Used to Address / Overcome:

No enough time, space, and assistance is a challenge. It seems difficult to get support (e.g. drawings of buildings) from campus organizations. The GA student needs computer and space for research but I could not provide.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

Due to time limit, the onsite validation was not performed.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

The team has been always preforming research in sustainability and energy efficiency. Its long research goal is to understand the underlying energy mechanism of various building structure elements, develop cheap but robust instruments for professionals in both academia and industry, and eventually aid in building sustainability. The results from this research help the team accumulate experimental data and then attract external research funds from ORAU,

TDOT, and possibly NSF to maintain our research progress and enhance the research and education role of UTC in energy sustainability field. Particularly, without the award, we would not be able to purchase equipment and materials to produce preliminary data which is required for most proposals. All these helped the PI and Co-PI develop their capability in the research field.

Students Impacted

With the research funds from CEACSE, we offered scholarship to a female master student Raghda Mohamed on the project. She has been supported to learn Building Information Modeling (BIM) for building retrofitting application. She started from knowing little/nothing and now is an expert in BIM use. She used BIM to model one campus building and do retrofitting analysis. With the obtained research results, we have submitted posters to *research dialogue* and *technology symposium* at UTC. We are planning to submit a paper to ASCE conference in Fall 2018.

Community and Broader Impacts

Though significantly improved, Chattanooga, as one of the "dirtiest" U.S. cities identified by EPA in 1969, still has much space to be healthier and environmentally cleaner through building sustainability programs in view of its large body. Our department is attempting to catch up this optimal opportunity to contribute to better local environment and enhance energy efficiency in commercial buildings. Our department and the team have tried to contact various funding agencies and potential collaborators including private foundations, local city, non-profit organizations and major research universities to enhance our research capability in this promising domain.

Work products reduced to practice; provide a bibliographical entry where appropriate

1. Yuan J, Li L, **Wang E,** Skibniewski M (2018). Examining Sustainability Indicators of Space Management in Elderly Facilities---A Case Study in China. Journal of Cleaner Production (Under Revision)
2. **Wang E** (2017). Decomposing core energy factor structure of US commercial buildings through clustering around latent variables with Random Forest on large-scale mixed data. Energy Conversion and Management 153: 346-61.
3. **Wang E,** Forst J, Alp N, Wang X (2018). Optimizing business operation strategies under uncertainties---A simulation approach. Advances in Intelligent Systems Research (CJ) 151: 34-37.
4. Mohamed R, **Wang E,** Wang X (2018). Utilizing BIM for cost estimating in retrofit project (Drafted).
5. Cash M, **Wang E,** Wang X (2018). Building Information Modeling for Nonresidential Construction---An Industry Perspective, 2018 2nd International Conference on Applied Mathematics, Modeling and Simulation, Aug 26-27, 2018.
6. **Wang E,** Mao P, Chen M, Zhang X, Li L (2017). Climate effects in data envelopment analysis for residential energy performance benchmarking---An empirical case validation. 2018 ASCE-CRC Conference, New Orleans, Louisiana, USA, April 2-5, 2018.

Outreach & Collaboration

Met with Green Space director

EXTERNAL FUNDING

Proposal Submissions

1. ORAU: Collaborating with ORNL-DOE (PI),$200
2. UTC: Climate Effects in Residential Energy Performance (PI),$600
3. NSF: Deep Building Energy Benchmarking (PI), $282,560
4. TDOT: Retaining Wall Inspection (PI), $149,857

5. TDOT: Work zone Alert (Co-PI), $174,938
6. TDOT: Open graded Friction Course (Co-PI), $99,996
7. TC: Undergraduate Summer Research (Mentor PI), $5,200
8. NAHB: Homebuilding Education Leadership Program (PI), $100,000

Contracts / Awards Received

1. Oak Ridge Associated Universities: Collaborating with ORNL-DOE (PI), Travel Grant, $200
2. UTC: Climate Effects in Residential Energy Performance (PI), Faculty Development Grant, $600
3. Tennessee Department of Transportation: Retaining Wall Inspection (PI), $149,857
4. Tennessee Department of Transportation: Open graded Friction Course (Co-PI), $99,996
5. UTC: Undergraduate Summer Research (Mentor PI), $5,200
6. First Place in Reusable Abstractions of Manufacturing Process (RAMP) National Competition (Team Member, NIST, NSF, ASTM, ASME), Led by Dr. Chris Yuan at Case Western Reserve University

Sponsored Program Capacity Building Activities

Attended ASCE conference in Louisiana

Attended Technology Symposium and Research Dialogue

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

We will by apply for external grant to continue with the research direction soon.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

None.

What barriers (if any) do you face to reach these next goals?

None.

FINANCIAL ACCOUNTING

Total Award Amount: $49,902.00

Cumulative Expenditures: $46,415.00

Remaining Award Amount: $3,487.00

Appendix C

Awardee Project Reports

Extended from Previous Award periods into FY 2018

Dr. T. Daniel Loveless, Lead PI

Project Title: “Supplemental Award: Stochastic Modeling of Charge Trapping and Emission in Emerging Semiconductor Technologies”

Award Start - End Date: 07/01/2017-06/30/2018

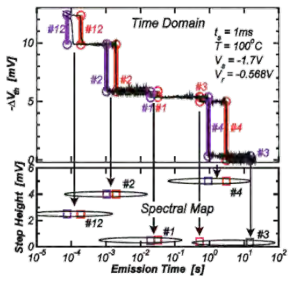
Non-Technical Summary:
The introduction of disruptive semiconductor technologies has created new reliability concerns for integrated circuits and systems. This supplemental award was used to design a technique for the measurement of stochastic time-dependent defects in advanced semiconductors devices such as the multi-gate FinFET. The measured stochastic behavior can be used in statistical reliability models for time-domain simulation of degradation and improved lifetime predictions. This work was conducted in collaboration with Dr. Michael King from Sandia National Laboratories.

Stochastic Modeling of Charge Trapping and Emission in Emerging Semiconductor Technologies

Technology Area of Interest: Urban Systems & Defense

OVERVIEW

- Discover emerging electronics reliability mechanisms
- Correlate device reliability with system behavior
- Create COMPACT stochastic
- reliability models suitable for time-domain circuit simulation
- Develop method for assessing Reliability at the physical layer (in-situ measurement of operational reliability)



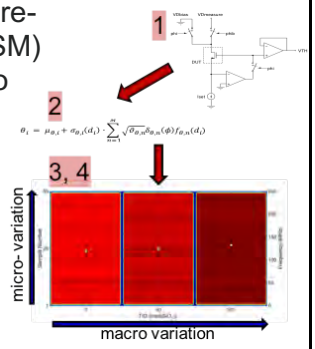
Grasser, Reisinger, et al., 2010

OPERATIONAL CAPABILITY PROVIDED

- Enhanced understanding of time-dependent reliability mechanisms
- Stochastic compact models for reliability simulations
- Non-invasive method for in-situ assessment of operational reliability and performance
- Applications in Reliability, Radiation Effects, Internet-of-Things, Exascale Computing, Security, and Trust

PROPOSED TECHNICAL APPROACH

- Develop Fast Measure-Stress-Measure (MSM) method applicable to small geometry semiconductors
- Enhance compact models with measured stochastic behavior for simulation of circuit and system



Collaborators include Sandia National Labs (devices) and Vanderbilt University (radiation effects)

OTHER INFO

ROM Cost & Schedule

- Period of Performance: 12 months.
- Cost: $3,581

Deliverables

- Monthly and Final Reports
- Participation in the 2018 UTC Research Dialogues
- Submission of an extramural proposal
  - NSF CAREER ($500,000), July 2018
  - Currently seeking appropriate programs within Dept. of Defense
- 2 Paper submissions to a peer-reviewed conference
  - Fast Measure-Stress-Measure (MSM) used to evaluate 22 nm PDSOI, 14 nm bulk FinFET, and 14 nm BOTS (presented at the 2018 IEEE NSREC)
  - In-situ measurement (presented at the 2018 IEEE NSREC)
  - Journal submission to IEEE Transactions on Nuclear Science, July 2018

Corporate Information

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Fax: (423) 425-1732
Email: daniel-loveless@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The goal of the research plan was to gather preliminary data on advanced (sub-32 nm technology nodes) FDSOI and/or FinFET devices using time-dependent defect spectroscopy (TDDS) [1] for developing a stochastic model of the random behavior of charge trapping and emission from atomistic defect centers. *With CEACSE 2016/2017 funding, the PI successfully 1) developed a time-domain defect spectroscopy (TDDS) instrument for measurement of sub-microsecond time-dependent defects, and 2) developed an analytical model for describing the stochastic behavior of time-dependent reliability effects.* The funding provided in the supplemental award was used to support a student researcher as a liaison to Sandia National Laboratories, and for obtaining preliminary data for population of the analytical model. The instrument was delivered to Sandia National Laboratories for integration into their advanced devices and reliability measurement capability. Sandia used the instrument to perform the measurements on 32 nm SOI and 14 nm FinFET devices and sharing data with UTC for population of the analytical model.

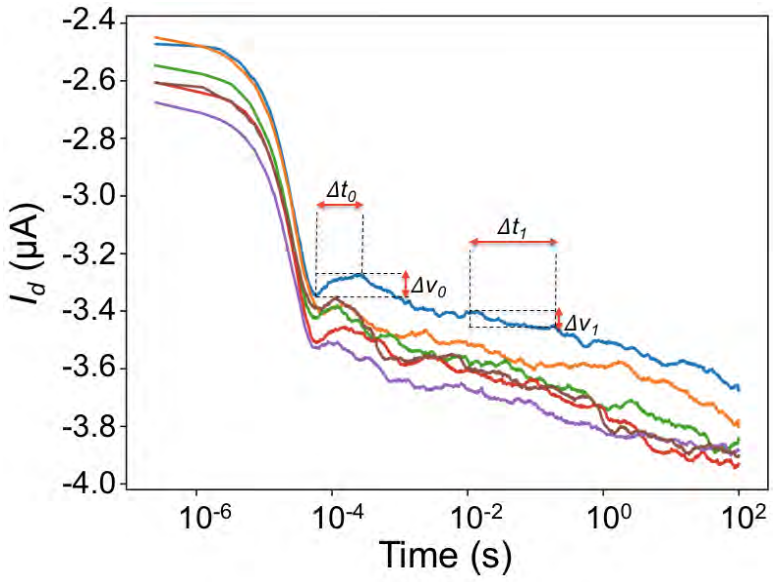


Figure 1. Recovery transients (I_d) at threshold in 32 nm SOI PMOS devices following a 10 second stress period at 130°C (V_{GS}=-1.5V, V_{DS}=0V).

Task 1. Figure 1 shows preliminary results from the TDDS method designed to capture the current near threshold. Recovery transients for six PMOS devices fabricated in a 32 nm SOI process are shown following 10 seconds of elevated temperature stress at 130 °C. The gate-to-source and drain-to-source bias voltages were -1.5 V and 0 V, respectively. The transients show discrete changes over time corresponding to the emissions of trapped charged particles. Each charge emission results in a voltage step (Δv_n)-emission time (Δt_n) pair that is related to the location and type of defect. However, the current technique has significant limitations at timescales less than 1 μsec. Future work will employ a method to directly measure the threshold voltage with fast-response operational amplifiers (which are required due to the inability to measure the threshold voltage in the time domain directly), minimizing parasitic elements that can contribute to measurement limitations and improve the bandwidth. This technique will allow for the capture of sub-1 μsec recovery threshold voltage transients, providing new insight into reliability recovery mechanisms.

Task 2. The general approach is to model any given parameter of transistor *i* as a random variable ϑ_i given by (1)

$$\theta_i = \mu_{\theta,i} + \sigma_{\theta,i}(d_i) \cdot p(d_i, \phi), \theta_i \in \{\theta_1, \ldots \theta_M\} \quad (1)$$

where $\mu_{p,i}$ and $\sigma_{p,i}(d_i)$ are the mean and standard deviation of the i^{th} transistor at location d_i on die ϕ, and p is the corresponding stochastic process that can take the form of an appropriate statistical distribution [2]. In this way, each parameter can be modeled using a generic approach that enables large-scale transparent simulations rather than through parametric sampling approaches through embedded behavioral compact models (though compact models will eventually be used to inform initial stochastic models and determination of the stochastic parameter *p* in the absence of data). Moreover, this approach will allow for the use of Bayesian inference to derive posterior probabilities improved with measured data. Though, initial models were created without the need for data, thus mitigating risk associated with device procurement and experimental measurement.

Recent work in the modeling of process variability has shown that by using a stochastic based formulation of necessary process parameters, a generalization of any finite number of electrical parameters θ_i can be described by a series expansion of uncorrelated random variables with deterministic functions [2]. For example, if $p(d_i, \phi)$ is a Gaussian process, then through Karhunen-Loève expansion, *M* terms of equation (1) can be expressed as (2)

$$\theta_i = \mu_{\theta,i} + \sigma_{\theta,i}(d_i) \cdot \sum_{n=1}^{M} \sqrt{\vartheta_{\theta,n}} \delta_{\theta,n}(\phi) f_{\theta,n}(d_i) \quad (2)$$

where $\delta_{p,n}(\phi)$ is a vector of uncorrelated Gaussian random variables, and $f_{\theta,n}(d_i)$ and $\vartheta_{p,n}$ are the eigenfunctions and eigenvalues, respectively, of the covariance matrix of $p(d_i, \phi)$ [2]. In other words, each parameter is describable as a random variable weighted by the distance d_i away from the reference (e.g., the origin of the die ϕ). Moreover, this approach allows for expansion to any spatial domain including die, chip, and system levels and has the potential to facilitate reliability assessment of large distributed applications with joint probability models. Monte-Carlo analysis of localized basic circuit parameters such as current, voltage, and timing [3] may also be used in this context, allowing for sensitivity analyses of the modeled elements to any statistical parameter of interest.

This approach will be expanded with the use of Bayesian inference[4][5], which derives the probability after evidence has been observed. As the initial models described by (1) and (2) will be derived from simulation data from predictive models and early manufacturing PDKs, the use of Bayesian inference will allow for refinement of the stochastic parameters based on new evidence gathered or measured. Thus, following the measurement of data *y* assumed to be representative of θ_i, one can write the posterior distribution of θ_i that depends on measurement *y* as (3)

$$p(\theta_i|y) = p(y|\theta_i)p(\theta_i)/p(y) \quad (3)$$

where $p(\theta_i)$ is the prior distribution of θ_i, $p(y|\theta_i)$ is the likelihood function of θ_i, and $p(y)$ is the probability function of measured data *y*. This approach will allow the posterior probabilities to be adjusted based on new data; this is particularly important, as reliability data is generally limited before technology release. Then, predictive distributions for any quantity *z* that may depend on θ_i (e.g., leakage current based on threshold voltage variation) can be derived as (4).

$$p(z|y) = \int p(z|\theta_i)p(\theta_i|y)\, d\theta_i \quad (4)$$

This stochastic approach will be used to model the dominant reliability failure mechanisms in FinFET devices. Then, the model will be generalized such that any number of chip level parameters (extracted from measurements as shown in Figure 1) can be included to model system level reliability of distributed systems, such as in IoT or sensor networks.

The preliminary data gathered from the CEACSE 2016/2017 funding as well as the 2017/2018 supplemental was used to support a submission to the NSF in July 2018 via the CAREER program.

References:

[1] T. Grasser, K. Rott, H. Reisinger, P. Wagner, W. Goes, F. Schanovsky, "Advanced Characterization of Oxide Traps: The Dynamic Time-Dependent Defect Spectroscopy," Proc. International Reliability Physics Symposium (IRPS), pp. 2D.2.1-2D.2.7, 2013.

[2] A. Zjajo (2014). Stochastic Process Variation in Deep-Submicron CMOS. Springer Netherlands.

[3] R. Hussin, S. M. Amoroso, L. Gerrer, B. Kaczer, P. Weckx, J. Franco, A. Vanderheyden, D. Vanhaern, N. Horiguchi, and A. Asenov, "Interplay Vetween Statistical Variability and Reliability in Contemporary pMOSFETs: Measurements Versus Simulations," IEEE Trans. Electron Devices, vol. 61, no. 9, pp. 3265-3273, Sept. 2014.

[4] A. Vehtari and J. Ojanen, "A survey of Bayesian predictive methods for model assessment, selection, and comparison," Statistics Surveys, vol. 6, pp. 142-228, 2012.

[5] D. Spiegelhalter and K. Rice, "Bayesian Statistics," Scholarpedia, vol. 4, no. 8, pp. 5230, 2009.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Perform TDDS on 14 nm FinFET devices. Use TDDS data to propagate analytical stochastic model.	1) Designed and fabricated a fast measure-stress-measure (MSM) instrument to observe both stress-induced degradation and defect recovery mechanisms in emerging sub-14nm CMOS technologies at 1 µsec timescales. Oct. 2018. 2) Verified MSM instruments electrical functionality. Dec. 2018. 3) Delivered instrument to Sandia National Laboratory for testing of 14 nm Bulk and SOI FinFET devices. Oct. 2018. 4) Performed reliability and radiation experiments at Sandia National Laboratory. Jan. 2018. 5) Design stochastic model based on measured data. July 2018. 6) Paper presented at the IEEE Nuclear, Space and Radiation Effects Conference (NSREC) in Kona, HI, July 2018. 7) Journal article submitted to IEEE Transactions and Nuclear Science (TNS). July 2018.

Challenges & Strategies Used to Address / Overcome:

While the basic function of the TDDS/MSM instrument allowed for general time-domain measurements, several issues were uncovered: 1) the time sensitivity is still limited to approximately 1 usec (an additional board with decreased trace impedance is required for further improvement), 2) the modes allowing for rapid change between stress and measure were non-functional (manual configuration was used but limited the number of devices

measured). The measurements were supplanted with additional measurements using standard fast sample techniques. Such data allowed for a conference presentation and journal article submission.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

See above.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

This work was instrumental in the completion of a proposal ($500,000) to the NSF CAREER program in July 2018. Preliminary data obtained from this effort was used directly in the program. The program also resulted in 1 paper and 1 conference presentation, and a national collaboration with industry leaders.

Students Impacted

Matthew Joplin: M.S. completed in Aug. 2018

Community and Broader Impacts

None

Work products reduced to practice; provide a bibliographical entry where appropriate

None

New inventions reduced to practice and when they will be formally disclosed;

None

Outreach & Collaboration

A collaboration with Sandia National Laboratories was established through this work.

EXTERNAL FUNDING

Proposal Submissions

NSF CAREER, $500,000, July 2018.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

Work was presented to program officers at DTRA, NASA, and the AF in May 2018. The work was well received, and discussions for potential funding are ongoing.

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

This supplemental award allowed for the completion of the TDDS instrument and early design of a stochastic model for describing the reliability behavior. The measurement technique and models will be refined in subsequent years to improve both experimental capabilities as well as improve models for reliability assessment. The research is also directly connected to other

programs in security, IoT, etc. The resulting measurement capability will be leveraged for improvement of current laboratory settings. Further, the collaborations built through this funding will help in development of additional programs and will strengthen UTC's presence in an international research setting.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

Collaborative opportunities in communications and security (Reising), Urban Systems (Sartipi), IoT (SimCenter), and others.

Tell us anything else we should know about this work not described above.

N/A

What barriers (if any) do you face to reach these next goals?

My current research capacity in terms of physical space and personnel is at maximum. Additional resources (lab space, post-doc, etc.) will be required within the next 2 years in order to maintain current growth rate.

FINANCIAL ACCOUNTING

Total Award Amount: $3581.00

Cumulative Expenditures: $3581.00

Remaining Award Amount: $0.00

Dr. Dalei Wu, Lead PI

Project Title: “Supplemental Award: Multiscale Serviceability Analysis and Assessment of Urban Infrastructure”

Award Start - End Date: 07/01/2017-06/30/2018

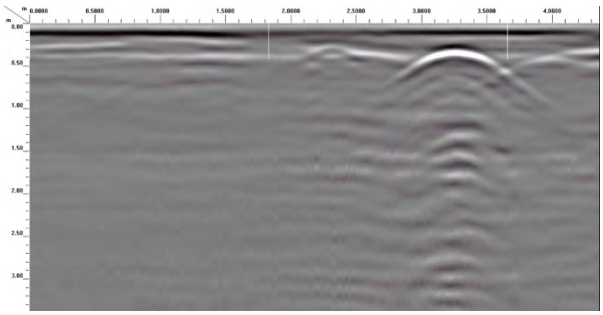
Non-Technical Summary:
The project was primarily targeted at developing a new multi-scale structural health monitoring system over Big-Data platform (MS-SHM-BD) to monitor and evaluate the serviceability of large-scale civil structures. Under the sponsorship of supplemental CEACSE funding, the team has been able to complete the major research goals and tasks of the project. The major outcome and impacts of the year 07/01/2017 – 06/30/2018 are:

- A demo was given in Smart Cities Connect Conference & Expo 2018, and the related project "Underground Infrastructure Sensing" was awarded as one of the 50 global most innovative smart city projects in the conference.
- Total 2 graduate students and 6 undergraduate students have been involved in the project.
- Five research papers have been published, including one journal paper and three conference papers. Two conference presentations have been provided.
- The team has submitted seven research proposals to NSF, NIST, and TDoT.

Multiscale Serviceability Analysis and Assessment of Urban Infrastructure

Technology Area of Interest: Urban Science

RESULTS



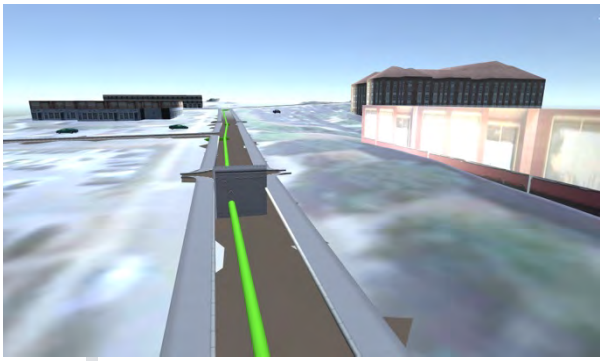


Figure 1: Underground pipeline monitoring and mapping

OPERATIONAL CAPABILITY PROVIDED

This project aims to develop a multi-scale structural health monitoring system over Big-Data platform (MS-SHMM-BD) to monitor and evaluate the serviceability of large-scale civil structures. The fundamental results of this project could help develop transformative techniques that can lead to improved safety and performance of the nation's urban infrastructure.

PROPOSED TECHNICAL APPROACH

Aiming to evaluate the structural health status of bridges and pipelines, a nationwide bridge/pipeline database survey, global structural integrity analysis, and component structural reliability analysis were performed by using methodologies of machine learning, signal processing, structural modeling and simulation, fatigue analysis, and Bayesian network. Specifically, the following research activities have been carried out.

- Stage 1: nationwide bridges/pipelines database survey.
- Stage 2: a global structural integrity analysis.
- Stage 3: localized structural component reliability analysis.
- Stage 4: Bayesian network based synthesis of component reliability

BUDGET AND SCHEDULE

Total Budget:	$95,610
Actual Used:	$84,580
Supplement award:	$10,000
Balance:	$ 0

Total period of performance is 12 months;
Stage 1 : Months 1-3
Stage 2 : Months 4-6
Stage 3 : Months 7-9
Stage 4 : Months 10-12

Deliverables:
Monthly Technical Report: Describing data processing methods, techniques and results that were developed or improved.
Progress/Status Report: Final Report

Organization Information:
UTC-SimCenter, UTC-CECS, Dr. Dalei Wu
735 Vine St, EMCS 315C
Chattanooga, TN 37403
Telephone: 423-425-4386
Email: dalei-wu@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The objective of the project was to develop a multi-scale structural health monitoring system over Big-Data platform to monitor and evaluate the serviceability of large-scale civil structures. Aiming to evaluate the structural health status of bridges and pipelines, a nationwide bridge/pipeline database survey, global structural integrity analysis, and component structural reliability analysis were performed by using methodologies of machine learning, signal processing, structural modeling and simulation, fatigue analysis, and Bayesian network. Specifically, the following research activities have been carried out. 1) Hadoop enabled data storage and analytics were explored. 2) Machine learning methods were studied for global structural integrity analysis and structural component reliability analysis. 3) Wireless networking (SDN) architecture was investigated for urban infrastructure monitoring and data delivery. The fundamental results of this project could help develop transformative techniques that can lead to improved safety and performance of the nation's urban infrastructure. Research findings in the year 07/01/2017 – 06/30/2018 were published in one journal paper, and one conference paper. Seven grant proposals were submitted to NSF, NIST, and TDoT for external funding applications. One NSF award has been received and ongoing: NSF (#1647175) "US Ignite: Collaborative Research: Focus Area 1: Fiber Network for Mapping, Monitoring and Managing Underground Urban Infrastructure," $299,884, 01/2017 - 12/2019. Another research fund to be received is

Rating and Inventory of TDOT Retaining Walls, Tennessee Department of Transportation (TDOT), $149,857, PI: Endong Wang, Co-PIs: Mbakisya Onyango, Weidong Wu, Dalei Wu, 10/2018 - 07/2020.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
With data acquisition, transmission and integration, bridges/pipelines database survey will be done to obtain a preliminary characterization of the safety level of major bridges and pipelines in the United States.	A Hadoop platform based on the CS cluster "Qbert" at the SimCenter has been used for data storage and analytics. A software-defined network (SDN) architecture has been proposed for delivery of urban infrastructure monitoring information. Various data analytics techniques such as missing data handling, variable transformation, data management optimization, and dimensionality reduction, etc. were employed.
Based on signal processing techniques, global structural integrity analysis of the targeted bridges/pipelines will be done to characterize and zone the potential damages.	A method for global structural integrity analysis has been developed by using measured structural resonance frequency and computed natural frequency. Ground penetrating radar (GPR) image processing techniques have been explored.
Localized structural component reliability analysis will be done to obtain a precise description about the specific heavily damaged zones/sections.	Two strategies of component reliability analysis, structural reliability analysis and observation-oriented method, have been investigated.

Component reliability analysis results will be synthesized to achieve a holistic characterization of the serviceability of the target bridges/pipelines.	Bayesian network was applied to generate a compact representation of joint probability distributions as global bridges reliability analysis.

Challenges & Strategies Used to Address / Overcome:

- Proper data for global structural integrity analysis targeted bridges/pipelines were missing. To overcome this challenge, collaboration with researchers from the University of Vermont was pursued to collect the needed data (e.g., GPR images).
- Students involved in this project lacked for background knowledge of infrastructure sensing, structural modeling and dynamics theory. Also, it was time-consuming for the team to figure out and get familiar with proper software tools for data processing and visualization. To overcome these issues, the PI and Co-PIs conducted training, provided study materials, and interacted with technicians to help students move forward with the project.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?

The research topic of this project is broad. At the outset of the project, it was expected to develop novel deep learning algorithms for nationwide bridges/pipelines database survey and component reliability analysis. Also it was expected to construct Bayesian network for integrity analysis. The team has formulated the idea of how to conduct research and then developed some preliminary framework. However, collecting real GPR data is an expensive and complex process. Also, the ground-truth data is scarce. What the team has learned is that data acquisition and integration is important and more research effort is needed.

IMPACT & OUTCOMES

Impact on the career(s) of the PI, the co-PIs, and key collaborators

PI: Dr. Dalei Wu, Assistant Professor in Computer Science. Co-PI: Dr. Yu Liang, Associate Professor in Computer Science; Dr. Yang Li, Professor in Computer Science, Dr. Farah Kandah, Assistant Professor in Computer Science, Dr. Joseph Kizza, Professor and Head of Computer Science. Key collaborators: Dr. Dryver Huston, Professor in Mechanical Engineering, UVM; Dr. Tian Xia, Associate Professor in Electrical and Computer Engineering, UVM

With the support of this supplemental grant, the PI and Co-PIs submitted sever research proposals collaboratively, and received one NSF grant (#1647175) "NSF US Ignite: Collaborative Research: Focus Area 1: Fiber Network for Mapping, Monitoring and Managing Underground Urban Infrastructure," UTC: $299,884, UVM: $298,525, 01/2017 - 12/2019, and one research grant from Tennessee Department of Transportation (TDOT), Rating and Inventory of TDOT Retaining Walls, $149,857, PI: Endong Wang, Co-PIs: Mbakisya Onyango, Weidong Wu, Dalei Wu, 10/2018 - 07/2020.

Students Impacted

The following students were involved in this project. With the support of this CEACSE project, most of them worked on this project with hourly pay.

Graduate students pursuing Ph.D degree in Computer Science: Maxwell Omwenga

Graduate students pursuing master degree in Computer Science: Stuart Eudaly, Maha Almaimani, Rabhu Bajracharya, Hector Suarez. Maha has graduated with a master degree in computer science.

Undergraduate students pursuing bachelor degree in Computer Science: Robert Slaughter, Dakila Ledesma, Christopher Davis, Alaykumar Patel, Suhail Arora, Austin Obyrne, Kane Kelley

Maha (female) published one conference paper as the first author.

Dakila Ledesma submitted one conference paper as co-authors.

Community and Broader Impacts

A project demo received broad attention from Smart Cities Connect Conference & Expo 2018. The related project "Underground Infrastructure Sensing" was awarded as one of the 50 global most innovative smart city projects in the conference. Students and participating municipal utility officials received educational experience in network-enabled sensing and urban infrastructure monitoring. Research results were shared through conference presentations, publications, and a website. The research conducted in this project was designed to determine methods of managing civil infrastructure in an urban setting, using network-enabled sensing and information processing techniques that are measurable, scalable and interoperable. Research results could enable cities to manage, maintain and grow their infrastructure in manners that improve service, sustainability and resilience, while reducing costs, energy consumption and wasted resources. Since many of the aging infrastructure lies in older cities, often subjected to economic distress and decay, this project has the potential to provide basic human needs and rights, and help to provide social justice through reliable low-cost provision of transportation, clean drinking water, functional storm and waste water sewers, heat, electricity and telecommunications. Additionally, there is significant potential for increased resilience and rapid effective management of recovery from disasters.

Work products reduced to practice; provide a bibliographical entry where appropriate

Journal papers:

- S. Mekid, D. Wu, R. Hussain, and K. Youcef-Toumi, "Channel Modeling and Testing of Wireless Transmission for Underground In-Pipe Leak and Material Loss Detection," International Journal of Distributed Sensor Networks, Vol. 13 (11), 2017.

Conference/workshop papers:

- Maha Almaimani, Dalei Wu, Yu Liang, Li Yang, Huston Dryver, and Tian Xia, Classifying GPR Images Using Convolutional Neural Networks. The 11th EAI International Conference on Mobile Multimedia Communications, Qingdao, China, June 21-22 2018.
- Hector Suarez, Li Yang, Dalei Wu, Securing GPR Data for Use in Smart Cities, IEEE Fourth International Conference on Big Data Computing Service and Applications (BigDataService), March 2018.
- Yu Liang, Dalei Wu, Dakila Ledesma, Zibin Guo, Virtual Tai -Chi System: A Smart-Connected Modality for Rehabilitation, IEEE/ACM CHASE, Washington DC, Sept. 2018.

Presentations:

- US Ignite Application Demo - Visualizing Underground Infrastructure in Augmented Reality, Smart Cities Connect Conference & Expo 2018: “Civil Infrastructure Serviceability Evaluation Based on Big Data,” by Drs. Dryver Huston, Dalei Wu, Yu Liang, March 2018, Kansas City MO.
- Civil Infrastructure Serviceability Evaluation Using Gpr-enabled Deep Learning, Drs. Yu Liang, Dalei Wu, MIT Engineering Mechanics Institute Conference, May 2018.

New inventions reduced to practice and when they will be formally disclosed;

A website has been created to make research results available to other researchers at minimal incremental costs.

https://gprusignite.com/

Outreach & Collaboration

- The team participated the meetings with professors from UTC, University of Vermont, and technicians and officers from The Enterprise Center, Chattanooga Department of Transportation, Chattanooga Public Works, EPB, and Tennessee American Water. The Enterprise Center held the meetings in the Center building.
- Research proposals were submitted by collaborating with professors and researchers from University of Tennessee at Chattanooga, University of Vermont, University of Tennessee at Knoxville, and Middle Tennessee State University.

EXTERNAL FUNDING

Proposal Submissions

- Self-Cleaning City Infrastructure for Prosperity and Health, submitted to NSF, $1,375,339, PI, Dryver Huston, Co-PIs: Dalei Wu, Lei Miao, Yu Liang, Tian Xia, February 2018.
- NSF CRI “CI-New: Collaborative Research: A Sandbox for Fostering Smart City Development,” submitted to NSF, $1,839,569, PI: Mina Sartipi, Co-PIs: Donald Reising, Dalei Wu, Farah Kandah, January 2018.
- CAREER: Towards Adaptive and Cognitive Wireless Video Sensor Networks for Enhanced Situational Awareness, submitted to NSF, $433,070, PI: Dalei Wu, July 2018.
- SCH: INT: RUI: Collaborative Research: ACTIVE -- Aging and Chronic disease/disability management with Tai-chi in an Individualized Virtual Environment, submitted to NSF, $903,279, PI: Yu Liang, Co-PIs: Zibin Guo, Amanda Clark, Dalei Wu, Nancy Fell, May 2018.
- NIST “A Fast, Reliable and Secure User Interface to Train and Equip Firefighters with Augmented Reality,” $524,205, PI: Dryver Huston, Co-PI: Li Yang, Dalei Wu, Yu Liang, Tian Xia, submitted in 01/2018.
- Rating and Inventory of TDOT Retaining Walls, submitted to Tennessee Department of Transportation (TDOT), $149,857, PI: Endong Wang, Co-PIs: Mbakisya Onyango, Weidong Wu, Dalei Wu, 10/2018 - 07/2020.
- A Cooperative Data-Driven Wrong-Way Driving Avoidance System (DWAS), submitted to Tennessee Department of Transportation (TDOT), $199,960, PI: Yu Liang, Co-PIs: Dalei Wu, Li Yang, Hong Qin, Sept. 2018.

Contracts/Awards Received

- NSF (#1647175) "US Ignite: Collaborative Research: Focus Area 1: Fiber Network for Mapping, Monitoring and Managing Underground Urban Infrastructure," $299,884, 01/2017 - 12/2019, PI: Dalei Wu, Co-PIs: Yu Liang, Li Yang.
- Rating and Inventory of TDOT Retaining Walls, submitted to Tennessee Department of Transportation (TDOT), $149,857, PI: Endong Wang, Co-PIs: Mbakisya Onyango, Weidong Wu, Dalei Wu, 10/2018 - 07/2020.

Sponsored Program Capacity Building Activities

- Dr. Wu participated in GWSW.
- Drs. Wu, and Dr. Liang attended Smart Cities Connect Conference & Expo 2018 and gave a project demo.
- Drs., Liang, Wu, Guo attended the Defense Innovation Technology Summit & Showcase in Tampa FL, October 2017, and gave a project demo.
- Dr. Liang attended MIT Engineering Mechanics Institute Conference, in Boston MA, May 2018, and gave a presentation.

- Drs. Wu and Liang and three students participated in 12-week GIGTANK accelerator program hosted by Co-Lab for startups developing business applications that thrive on low latency networks.

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?

The team will continue conduct in-depth study of the research topics identified in this CEACSE project. In the following year, we will focus on the development of generative models to expand our dataset. Field experiment is under preparation by collaborating with University of Vermont and interacting with utility officials.

The team will continue the collaborations that have been established through this CEACSE project to publish the generated research results, and submit external grant applications.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

Several smart city and public safety related projects including connected vehicles, railroad safety, fire fighting, and crime curbing, will be pursued by collaborating with UTC faculty and external researchers (Dr. Dryver Huston and Dr. Tian Xia from University of Vermont, Dr. Guirong Liu from University of Cincinnati, Dr. Zhongguo John Ma and Dr. Husheng Li from University of Tennessee at Knoxville, Dr. Yaohang Li from Old Dominion University, Mr. Richard Lusk from Oak Ridge National Laboratory, The Enterprise Center and other local organizations.)

Tell us anything else we should know about this work not described above.

N/A

What barriers (if any) do you face to reach these next goals?

Funding is needed to support students working on the identified research through this project

The teaching load of the PI and Co-PIs is high, leaving insufficient time for conducting research and supervising students.

FINANCIAL ACCOUNTING

Total Award Amount: $10,000.00

Cumulative Expenditures: $10,000.00

Remaining Award Amount: $0.00