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 2018-2019

OCTOBER 15, 2019

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UNIVERSITY OF TENNESSEE 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 PhD 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 FY2018, CEACSE marked its 13th year of growing UTC's first Center of Excellence into a critically important incubator for inquiry and experimentation across a diverse array of computational science and engineering endeavors. This report for FY2019 follows up our previous report with CEACSE's focused priority areas, highlights the ongoing strengths of its visionary leadership team, and notes greater impacts across a range of stakeholder groups. CEACSE comprises the indispensable factor that enables UTC to recruit, retain, and engage outstanding professors and equally outstanding students through research experiences for undergraduates up to and including PhD students.

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

Notable outcomes in FY2019 include these highlights:

- Dr. Hong Qin was awarded $359,971 for the NSF project entitled "REU Site: iCompBio - Engaging Undergraduates in Interdisciplinary Computing for Biological Research."
- Dr. Abdollah Arabshahi took over an NSF project entitled "RUI: Efficient Adaptive Backward Stochastic Differential Equation Methods for Nonlinear Filtering Problems," which remained at UTC when former UTC faculty Dr. Feng Bao relocated to Florida. The award totaled $124,995.
- Dr. Hong Qin was awarded $549,888 for the NSF project entitled "Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education."
- Drs. Anthony Skjellum, Don Reising, and Farah Kandah received $250,000 from the ORNL/UT/Launch Tennessee RevV program for collaborative R&D in Modeling, Simulation, and Engineering with International Maritime Security Associates, Inc..
- Drs. Anthony Skjellum and Craig Tanis received $450,097 from the National Science Foundation for collaborative work with Boston University on Heterogeneous HPC, titled " SPX: Collaborative Research: Intelligent Communication Fabrics to Facilitate Extreme Scale Computing."

- Drs. Anthony Skjellum and Craig Tanis received $100,000 from the Sandia National Laboratories for studies of Exascale Computing.
- Dr. Anthony Skjellum received $60,000 from the Lawrence Livermore National Laboratory for Fault-Tolerant HPC Research.
- Dr. Farah Kandah was awarded $499,663 from the National Science Foundation for the project entitled “CC* Networking Infrastructure: Advancing High-speed Networking at UTC for Research and Education,” to support 100Gbit/s networking to connect CEACSE computing and data resources with seven other campus R&D centers, enabling modeling and simulation work and accessibility across campus. These resources are being deployed in FY2020 and FY2021.
- Dr. Anthony Skjellum and team were awarded $392,235 from the National Science Foundation for “CC* Compute: A Cost-Effective, 2,048 Core InfiniBand Cluster at UTC for Campus Research and Education” to support a 2,048-core AMD-based HPC cluster. These resources are being deployed in FY2020.

Important technical advancements achieved in FY2019 include these highlights:

- Technical collaborations within SimCenter led to the creation of the “Digital Twins” Swimlane that launched on July 1, 2019, and has already received its first NSF funding for engineering curriculum development.
- UTC’s first virtual private cloud was procured and deployed with CEACSE support in the SimCenter to support High-Performance Computing and High-Throughput Computing
- UTC hosted a petascale computing workshop for approximately ten attendees. The workshop included instruction in MPI, Python, CUDA, software engineering best practices, and other core competencies in HPC.
- Dr. Francesca Leasi, as a result of a Faculty Initiation Award (details below), began a series of workshops called the Southeastern Computational School. The first annual workshop, hosted at UTC, brought in developers/instructors for the QIIME2 software, a microbiome bioinformatics platform used to solve a wide range of computational biology problems. The 25 attendees included faculty and students from 14 universities across the nation. The workshops will continue annually, with the aim of increasing educational opportunities and fostering new collaborations in computational biology.
- As a result of CEACSE funding, Dr. Azad Hossain convened the Inaugural Workshop of Southeastern Computational and Geospatial Environmental Hydrology, a multi-institutional group he founded with the help of Dr. Mustafa Altinakar at the University of Mississippi National Center for Computational Hydroscience and Engineering (NCCHE). The 28 attendees from UTC, NCCHE, and Tennessee Technological University found common ground in their research efforts and declared a shared vision for regional collaboration on federal funding opportunities and beyond. The next workshop will be held at NCCHE.

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

to invite an accomplished researcher in their field to speak at UTC. All lectures are public, and promising research collaborations have resulted from each one.

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

This document constitutes the Annual Report for Fiscal Year 2019 of CEACSE activities and efforts. On behalf of UTC, SimCenter, 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.

TABLE OF CONTENTS

Mission Statement i
Vision Statement i
Executive Summary iii
Table of Contents vii
Faculty & Staff 1
Students 17
Program Overview & Accomplishments 25
Budget and Schedule 7 38
Publications 43
External Funding (Grants & Contracts) 53
Overview of FY2020 Projects 59
Conclusion 67
Contact Information 69
Appendix A – Faculty Biosketches 71
Appendix B – Project Reports 147

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. Please see the **Leadership Contact Information and Bios** section for details of leadership personnel.

CEACSE FY2019 Awardees

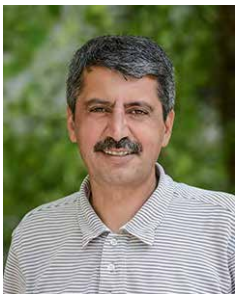
The following faculty and staff were integral to the strategic direction of CEACSE during the 2019–20 competition cycle, on both core and Faculty Initiation/Opportunity Awards. As noted below, these individuals served as a Lead PI and/or Co-Investigator on projects that advanced the CEACSE mission and vision. Biosketches for all faculty may be found in **Appendix A**.

Dr. Mo Ahmadi

Dr. Mohammad Ahmadi is a Guerry Professor in the Department of Management. His specialization is in Data Analytics, and he is the course coordinator of Statistics and Operations Management. He received his BS in Mechanical Engineering in 1968, his MBA in 1970, and his PhD in Management Science in 1976. He has been a consultant to firms in the southeast US. Most of his consulting work has dealt with operations research, statistical sampling, forecasting, and data analytic. He has published many articles in academic and professional journals such as *International Journal of Management, The International Journal of Business, Marketing, and Decision Sciences, SAM: Advanced Management Journal, Quality Assurance in Education, International Journal of Simulation Modeling,* and the *Scientific Journal of Administrative Development*. Cengage Publishing Company published his study guide/workbooks *Statistics for Business and Economics* and *Essentials of Statistics for Business and Economics*. His current work *Statistics for Business and Economics: A Study Guide and Workbook with Excel Instructions and Examples* is published by Kendall Hunt (2016). Please refer to Dr. Ahmadi's biosketch in **Appendix A** for more information.

Co-Investigator:
"Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design"

Dr. Abdollah Arabshahi



Dr. Abdollah Arabshahi is a SimCenter Research Professor. He received a BS (1982) in Civil Engineering and an MS (1985) and a PhD (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, *Journal Physics Letters A, Journal of Nanomaterials, Scientific Reports Journal, Journal of Royal Society of Chemistry Advances, 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.

Co-Investigator:
"Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels"

"Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities"

Dr. Jejal Reddy Bathi

Dr. Jejal Reddy Bathi is a Visiting Assistant Professor in the Department of Civil and Chemical Engineering. He received his BS (2000) in Chemical Technology from Osmania University, first M.S (2005) in Environmental Engineering from National University of Singapore and second MS (2007) in Environmental Engineering and PhD (2008) in Civil Engineering from the University of Alabama. Dr. Bathi's research includes understanding changing urban land development dynamics and their impacts on watershed hydrology and water quality. He has several peer-reviewed publications including journal articles, book chapters, technical reports, and national and international conference proceedings. He is a member of the American Society of Civil Engineers and the Association of Environmental Engineering and Science Professors. As Co-PI of CEACSE, Dr. Bathi has been simulating fate and transport of contaminants in surface water systems and also evaluating the impact of environmental pollution on microbiology in the surface waters. Please refer to Dr. Bathi's biosketch in **Appendix A** for more information.

Co-Investigator:
"Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems"

Dr. Jennifer Boyd

Dr. Jennifer Boyd is a Professor and Associate Department Head for the Department of Biology, Geology, and Environmental Science. She received a BS (1997) in Environmental Science/English (double major) from Allegheny College and an MA (2001), MPhil (2002), and PhD (2003) in Earth & Environmental Sciences from Columbia University. Her research includes plant ecophysiology, global change biology, biological conservation, experiential learning, and science writing. Dr. Boyd has authored 15 papers in refereed journals, most as first author or as co-author to a student. She and her students have given more than 40 presentations at research conferences and symposia. 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 CEACSE co-PI, Dr. Boyd has explored the use of computational tools to address ecological questions related to species abundance, with specific focus on species rarity. 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:
"Using Computational Tools to Understand the Fundamental Rules of Life"

Dr. Michael Danquah

Dr. Danquah is a full Professor and the Director of Chemical Engineering Program at UTC. He also serves as the Associate Dean for the College of Engineering and Computer Science. He is a Chartered Professional Engineer (CPEng), Chartered Scientist (CSci), and a Fellow of the Institution of Chemical Engineers (IChemE). He obtained his PhD from Monash University (Australia). Dr. Danquah's research focuses on the use of biomolecular engineering principles to develop targeted drug delivery, biosensing, and molecular separation systems. For his CEACSE grant, he investigated the molecular mechanisms governing aptamer-target binding to optimize applications for targeted drug delivery and biosensing. Dr. Danquah's research findings are well published and cited with over 230 peer-reviewed publications and conference proceedings and a current H-index of 35. He has served as a consultant to companies including agricultural, pharmaceutical and biofuels industries. Dr. Danquah is a member of the Board of Trustees of OA Publishing London, an Associate Editor of *BMC Biotechnology*, and an Editorial Advisory Board member of *Current Pharmaceutical Biotechnology*. His research has received several awards and recognitions including a Gold Medal award at the 2017 Word Invention Innovation Contest. He is a member of AIChE minority affairs community and faculty forum. Please refer to Dr. Danquah's biosketch in **Appendix A** for more information.

Lead PI:
"Kinetic and Computational Elucidation of Nucleic Acid Aptameric Binding Mechanism for Enhanced Molecular Targeting"

Dr. Vahid Disfani

Dr. Vahid Disfani has been an Assistant Professor of Electrical Engineering and the director of ConnectSmart Research Laboratory at the University of Tennessee at Chattanooga (UTC) since August 2017. He earned his PhD in Electrical Engineering from University of South Florida in 2015 and conducted research as a postdoctoral scholar at the University of California San Diego (UCSD) in 2015-2017. His research areas include power electronics, power system optimization and control, and grid integration of distributed energy resources (DERs). His publication record includes 19 journal papers (5 under review), 18 conference papers, and 3 technical reports that have been cited 370+ times. During his two-year postdoc at UCSD, he led tasks of research projects funded by California Energy Commission (CEC) and U.S. Department of Energy (DOE) for a total of $6.8M. At UTC, he served as PI on a research grant funded by Tennessee Valley Authority (TVA) for $33k and a CEACSE award for $96k, which his research team at UTC ConnectSmart Research Lab recently completed. He developed an urban charging market for electric vehicles to maximize the social welfare and minimize energy consumption and CO2 emissions in collaboration with UTC College of Business, Electric Power Board (EPB), and Chattanooga Area Regional Transportation Authority (CARTA). He currently collaborates as senior personnel in a recently funded NSF RET research grant on engineering and data analytics in smart cities for $596k.

Lead PI:
"Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design"

Dr. Ignatius Fomunung

Dr. Ignatius Fomunung is a Professor in the Department of Civil and Chemical Engineering, and Director of UTC's Center for Energy, Transportation and Environment (CETE). He received a BS (1987) in Civil Engineering from the Southeast University in Nanjing, China, an MSc in Physics (1995) from Clark Atlanta University, Atlanta, Georgia; an MS in Transportation Engineering (1996) from Georgia Institute of Technology (GaTech); and a PhD (2000) in Civil & Environmental Engineering from GaTech. His research includes transportation planning, transportation-air quality-energy analysis, traffic operations and safety, and atomic and molecular physics. Dr. Fomunung has authored more than 20 papers in refereed journals, as first author or as co-author, and has given 15+ presentations at conferences and symposia. His combined external funding as a PI while at UTC has totaled nearly $1.2 million, and nearly $4.5 million as Co-PI.

Lead PI:
"3D Drone Delivery Transportation Problem"

Dr. Arash Ghasemi

Dr. Arash Ghasemi is the director of civil infrastructure and research in the department of civil end chemical engineering. His area of interests includes geometric modeling and computational simulations. He is currently supervising two graduate students. His teaching and research are focused mainly on the area of structural engineering and transportation.

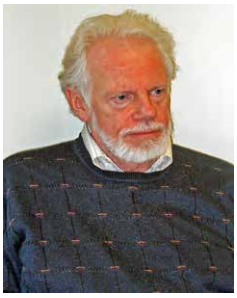
Co-Investigator:
"3D Drone Delivery Transportation Problem"

Dr. David Giles

Dr. David Giles is an Associate Professor for Biology, Geology and Environmental Science. He received a BA (2001) in Biology from Maryville College and a PhD (2008) in Biomedical Sciences with a concentration in Microbiology from East Tennessee State University. His research and involves assessing impacts of exogenous fatty acids on membrane composition and virulence of Gram-negative bacteria, with four publications on the topic since 2017. Dr. Giles uses microbiology, genetics, and biochemistry to investigate 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:
"Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation"

Dr. John R. Graef



Dr. John R. Graef is a Professor of Mathematics; he holds a PhD from Southern Illinois University. His research interests are in the areas of differential and difference equations, integral equations, impulsive systems, stability theory, fixed point methods, and applications to biological systems. In addition to 13 research monographs, one of which has just been nominated for the Doob Prize in Mathematics, Dr. Graef has authored or co-authored more than 475 papers in refereed journals. He has more than 130 co-authors from 21 foreign countries and the U.S. He has made more than 230 presentations at regional, national, and international conferences. He referees papers for more than 100 different journals and serves on the editorial boards of more than 25 journals. He was awarded a bronze medal by Masaryk University in Brno (Czech Republic) in 2013 for ``outstanding and beneficial work in the cultivation of letters and sciences." In 2015 he received the UTC Lifetime Research and Creativity award the first time the award was offered.

Co-Investigator:
"Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations"

Dr. Sumith Gunasekera

Dr. Sumith Gunasekera received the (Bachelor of Science with Honors) B.Sc. (Hons.) degree in Physics in 1995 from the University of Colombo, Sri Lanka (formerly known as Ceylon), and the (Doctor of Philosophy) PhD degree in Statistics in 2009 from the University of Nevada at Las Vegas (UNLV), NV, USA. Dr. Gunasekera joined the Department of Mathematics at The University of Tennessee at Chattanooga (UTC), Chattanooga TN, USA in 2009, and has been an Associate Professor of Statistics since 2015. Dr. Gunasekera has more than 10 years of collaborative, consulting, and methodological research experience in biostatistics, public health, biomedical, clinical, epidemiological, and social science research. His research interests include clinical trials, cluster trials, probabilistic disease modeling, stochastic models, longitudinal data analysis methods, predictive modeling, classical inference, Bayesian inference, non- and semi-parametric inference, generalized variable inference, reliability, survivability, design of experiments, stochastic process, spatial data analysis, computational statistics, and stochastic differential equations (SDEs). Dr. Gunasekera has published widely on a variety of topics in statistical and scientific journals, led workshops in different topics, and presented his research as a keynote, invited, and contributing speaker. He has received several awards for his published research articles. As a PI in a recently awarded CEACSE grant, Dr. Gunasekera has been developing modular high-performance computational resources as part of a web services framework called GeneralizedMultivariateYouden (GMY) that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers in the presence of missing and grouped, or pooled, data.

Lead PI:
"Estimating the Youden Index Under the Multivariate Roc Curve in The Presence of Missing Values of Mass Diseased and Healthy Biomarker Data"

Dr. Bradley Harris

Dr. Bradley Harris is an Assistant Professor in the Department of Civil and Chemical Engineering at UTC. He received his PhD (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.

Dr. Harris is also interested in engaging local community college students in chemical engineering through 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.

Co-Investigator
"Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation"

Dr. Ethan Hereth

Dr. Ethan Hereth is an HPC Specialist for the SimCenter at UTC. He received his PhD (2016) in Computational Engineering at UTC. He is in charge of designing, improving, and maintaining all associated hardware, as well as installing, testing, and maintaining sundry research software spanning many application areas. His research interests are in Computational Engineering with a focus on Computational Fluid Dynamics and 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. In September 2019, Dr. Hereth left the SimCenter for another position in the UT system. Please refer to Dr. Hereth's biosketch in **Appendix A** for more information.

Co-Investigator:
"Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities"

Dr. Azad Hossain

Dr. Azad Hossain is an Assistant Professor in the Department of Biology, Geology, and Environmental Science at the University of Tennessee at Chattanooga (UTC). He received his MS and PhD degrees from the University of Mississippi (UM) (2004 & 2008) in Geological Engineering and B.Sc. and M.Sc. degrees from the University of Dhaka, Bangladesh (1995 & 1998) in Geology. Dr. Hossain's research interests focus on the applications of GIS, Remote Sensing, and Spatial Analysis techniques in different areas of earth and environmental science including quantitative estimation of different geophysical variables in terrestrial and aquatic environments using remotely sensed data acquired in optical and microwave portions of the electromagnetic spectrum. Dr. Hossain published 5 invited book chapters, 11 peer reviewed articles, and 20 conference proceedings articles. He delivered more than 30 oral presentations and more than 20 poster presentations at different international, national, and regional conferences. Dr. Hossain served/currently serving as PI and Co-PI on several internal and externally funded research projects. Please see Dr. Hossain's biosketch in **Appendix A** for more information.

Co-Investigator:
"Using Computational Tools to Understand the Fundamental Rules of Life"

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 BS in Computer Science form the Hashemite University, Jordan in 2002, his MS degree in Computer Science from the University of Jordan in 2005, and his PhD 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 reviewed for 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.

Lead PI:
"STC3: A Smart Trust-based Connected Autonomous Collaborative Communities"

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 BS in Zoology and Psychology and her PhD in Zoology 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:

"Using Computational Tools to Understand the Fundamental Rules of Life"

Dr. Lingju Kong

Dr. Lingju Kong is a UC Foundation Professor in the Department of Mathematics at UTC. He received his PhD in Mathematics in 2005 from Northern Illinois University. He was a Co-PI for an NSF REU grant. His expertise and research interests lie in the general areas of ordinary and partial differential equations, epidemic models, online social networks, and other related topics. He has co-authored 3 research monographs and published over 145 research papers in refereed journals. According to the data from Google Scholar, his work has been cited over 1900 times. He has been invited to give talks at national and international conferences. He currently serves on the editorial board of one international mathematical journal and he has been invited to referee papers for numerous mathematical journals. Please refer to Dr. Kong's biosketch in **Appendix A** for more information.

Lead PI:

"Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations"

Dr. Francesca Leasi

Dr. Francesca Leasi is an Assistant Professor for the Department of Biology, Geology, and Environmental Science. She received a MS (2002) in Biology, and PhD (2007) in Evolutionary Biology from the University of Modena and Reggio Emilia, Italy. Her research and academic interests include macroecology, evolutionary biology, and patterns of diversity and distribution of microscopic organisms. She has authored over 35 publications on these areas in refereed journals, including *Molecular Ecology* and *Proceedings of the National Academy of Sciences*. As a PI on a faculty initiation CEACSE award, Dr. Leasi has been exploring the biodiversity of local microscopic communities from freshwater environments located in Tennessee. The project has attracted the

interest of undergraduate and graduate students currently working in Leasi's lab. She also regularly presents her research at national international conferences, including the International Meiofauna Society, Society of Integrative Biology, Ecology and Evolution Conference.

Lead PI:
"Development and application of bioinformatics pipelines and theoretical models to predict microbiome biodiversity in response to environmental stressors"

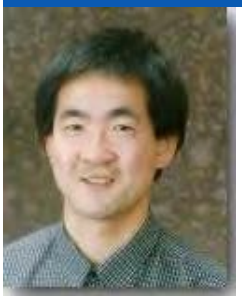
Dr. Andrew Ledoan

Dr. Andrew Ledoan currently works as Associate Professor of Mathematics at The University of Tennessee at Chattanooga. He received his BS (1993) in Electrical Engineering from San Jose State University, MS (2001) in Mathematics from San Jose State University, MS (2006) in Mathematics from University of Illinois at Urbana–Champaign, and PhD (2007) from University of Illinois at Urbana–Champaign. Before working in academia, Dr. Ledoan worked as Senior Software Engineer at Trimble Navigation, where he designed firmware for GPS receivers for navigation, tracking, data collection, and timing applications. Dr. Ledoan's current research is in Number Theory, Probabilitym and Mathematical Statistics. He has authored/co-authored 24 articles in peer-reviewed journals, and five articles are currently under review for publication. Dr. Ledoan is the PI of an NSF funded REU Site in Mathematical Analysis and an MAA Dolciani Mathematics Enrichment Grant for the project Chattanooga Math Circle. At UTC, he has mentored 15 undergraduate students, 13 of whom are REU students, and five of whom are currently pursuing PhDs in Mathematics at top R1 institutions. In addition, he has mentored three MS students. As a Co-PI on one CEACSE award, Dr. Ledoan has produced three articles. One of these articles is joint with his current PhD student, who will be presenting the research findings at the next AMS Sectional Meeting's AMS Special Session on Probabilistic Methods in Geometry and Analysis (University of Virginia, March 13-15, 2020). Please refer to Dr. Ledoan's biosketch in **Appendix A** for more information.

Co-Investigator:

"Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations"

Dr. Yu Liang



Dr. Yu Liang is an Associate Professor in the Department of Computer Science and Engineering of UTC. His funded research covers big-data and cloud computing, modeling and simulation, high-performance scientific and engineering computing, numerical linear algebra, processing and analytics of large-scale sensory data, and computational mechanics. His research has appeared in various journals; book or book chapters; and refereed conference, workshop, and symposium proceedings. Currently, Dr. Liang has four NSF-funded projects. He owns one technical pattern that is registered at the Univ. of Tennessee Research Foundation (UTRF). Dr. Liang serves on the International *Journal of Security Technology for Smart Device* (IJSTSD), *Journal of Mathematical Research and Applications* (JMRA), and *Current Advances in Mathematics* (CAM) as an editorial board member. Please refer to Dr. Liang's biosketch in **Appendix A** for more information.

Co-Investigator:
"Analyzing Bioimage Big Data with Deep Learning Neural Networks"

Dr. Daniel Loveless

Dr. Daniel Loveless is a UC Foundation Associate Professor of Electrical Engineering at UTC. He received a BS in electrical engineering from Georgia Institute of Technology, Atlanta, Georgia, in 2004 and MS and PhD 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 90 articles in peer-reviewed journals, has been cited over 1580 times, and is a Senior Member of IEEE. His honors include the recently awarded 2019 Nuclear and Plasma Sciences Society (NPSS) Radiation Effects Early Achievement Award, five best conference paper awards, the IEEE NPSS Graduate Scholarship Award for recognition of contributions to the fields of nuclear and plasma sciences, and the Georgia Tech Alumni Association Scholarship. Please refer to Dr. Loveless's biosketch in **Appendix A** for more information.

Lead PI:

"Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications"

Mbakisya Onyango

Dr. Mbakisya Onyango is UC Foundation Associate Professor in Civil and Chemical Engineering Department at the University of Tennessee at Chattanooga (UTC). She graduated with a PhD in Transportation Engineering from Kansas State University in 2009 and Master's in International Highway Engineering from the University of Birmingham in the United Kingdom. At UTC she teaches civil engineering undergraduate and graduate classes and conducts research in transportation and construction materials. Since joining UTC in 2010, she has attracted research funding to the amount of $ 2.4 million as PI or Co-PI including funding from CEACSE, TDOT, and NSF. Ahe has over 40 journal publications and conference proceedings. She has advised over 100 undergraduate students and supervised 10 graduate students' theses. Please refer to Dr. Onyango's biosketch in **Appendix A** for more information.

Co-Investigator:
"3D Drone Delivery Transportation Problem"

Joseph Owino

Dr. Joseph O. Owino is a Professor of Civil Engineering and the department head for Civil and Chemical Engineering. Dr. Owino's research interests are in the areas of structural health monitoring, Non-destructive evaluation of civil engineering materials and analysis and design of pavement structures and Finite Element Method (FEM). Dr. Owino received his PhD from Georgia Institute of Technology. Dr. Owino is a registered professional engineer in the state of Tennessee. He currently teaches courses in Engineering Mechanics and Structural Analysis. He is affiliated with American Society of Civil Engineers (ASCE), American Society of Engineering Education (ASEE) and National Society of Black Engineers (NSBE). Dr. Owino has authored or co-authored over 20 journal papers and more than twenty presentations at research conferences and symposiums. His combined external funding as PI or co-PI while at UTC has totaled nearly $2 million. Please refer to Dr. Owino's biosketch in **Appendix A** for more information.

Co-Investigator:
"3D Drone Delivery Transportation Problem"

Dr. Soubantika Palchoudhury

Dr. Soubantika Palchoudhury is an Assistant Professor in the Civil and Chemical Engineering department at UTC. She received her PhD (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 interests include nanochemistry, biohybrid nanoarchitectures, semiconductor nanocrystals for photovoltaics, environmental nanoscience, and material characterization, especially transmission and scanning electron microscopy. Dr. Palchoudhury has authored 30 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. 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: "Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels"

Dr. Jared Pienkos

Dr. Jared Pienkos is an Assistant Professor for the Department of Chemistry and Physics. He received a BA (2009) in Chemistry/Math (double major) from Hamilton College. He then received his PhD from the University of Virginia (2014), working under Dr. Walter D. Harman where he developed synthetic methodology utilizing dearomatization reagents. Following graduate school, Dr. Pienkos completed a postdoctoral position at Furman University, working with Dr. Paul S. Wagenknecht to investigate the metal-to-metal charge transfer in Fe(II)/Ti(IV) compounds. Dr. Pienkos has authored 13 papers in peer reviewed journals, including *Journal of the American Chemical Society*, *Inorganic Chemistry*, *Organometallics*, and *Dalton Transactions*. Currently, he has a research group of six undergraduate students and one high school

student. As a PI on a mini-CEACSE award and a CEACSE award, Dr. Pienkos has been investigating transition metal alkynyl compounds with the hopes of generating new catalysts and molecular devices (e.g., organic light emitting diodes). Results of this work will be presented at the regional chemistry meeting, SERMACS, and the PI plans on taking three students to the National ACS meeting in Philadelphia to present this work. Please refer to Dr. Pienkos's biosketch in **Appendix A** for more information.

Lead PI:
"Exploiting Alkynyl Titanocenes for Carbon-Carbon Bond Formation"

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). Please refer to Dr. Qin's biosketch in **Appendix A** for more information.

Lead PI:
"Analyzing Bioimage Big Data with Deep Learning Neural Networks"

Co-Investigator:
"Estimating the Youden Index Under the Multivariate Roc Curve in The Presence of Missing Values of Mass Diseased and Healthy Biomarker Data"

"Using Computational Tools to Understand the Fundamental Rules of Life"

Dr. Donald Reising

Dr. Donald R. Reising is an Assistant Professor of Electrical Engineering at UTC. He received his BS degree in Electrical Engineering from the University of Cincinnati in 2006. He received his MSE.E. (2009) and PhD (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.

Co-Investigator:
"Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications"

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 BS in Electrical Engineering from Sharif University of Technology, Tehran, Iran, in 2001 and her MS and PhD 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:
"Improving Post-stroke Management Efficiency and Patient Outcomes through Analytics"

Co-Investigator:
"STC3: A Smart Trust-based Connected Autonomous Collaborative Communities"

"Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design"

Joey Shaw

Joey Shaw earned his MS (2000) and PhD (2005) degrees from the University of Tennessee, Knoxville. In 2005, he accepted the position of Assistant Professor in the Department of Biology, Geology, and Environmental Sciences at UT Chattanooga. He was awarded a University of Chattanooga Foundation professorship along with tenure and promotion in 2010. In 2015, he was promoted to the rank of Full Professor and in 2016 he was inducted into the university's Council of Scholars. He has successful research programs in molecular systematics of plants, biodiversity inventories, and herbarium/museum curation, digitization, and modernization. Highlights of his career include being first author of two of the top five most highly cited papers in the *American Journal of Botany*. He has over 4000 career citations and he has coauthored over 30 papers in *AJB*, *Molecular Phylogenetics and Evolution*, *Journal of Ecology*, *Journal of Systematics and Evolution* and many more in regional journals. He is an author and editor of the *Guide to the Vascular Plants of Tennessee*.

As a lead investigator, he has secured over $2.4 million in funding, largely from state and federal agencies. He is active in state, regional, and national organizations and has held elected positions on the Southern Appalachian Botanical Society, Tennessee Academy of Sciences, and he served as President of the Association of Southeastern Biologists. His largest outreach activity is organizing the annual Spring Wildflower Pilgrimage in the Great Smoky

Mountains National Park, which brings more than 100 experts together with over 1000 members of the public from 35 states to engage in biodiversity education and public outreach. Please refer to Dr. Shaw's biosketch in **Appendix A** for more information.

Co-Investigator:

"Analyzing Bioimage Big Data with Deep Learning Neural Networks"

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:
"Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities"

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 MS in Computer Science from Tulane University in 1997 and 1998, respectively. He received his PhD 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:
"Analyzing Bioimage Big Data with Deep Learning Neural Networks"

Dr. Endong Wang

Dr. Endong Wang is an Assistant Professor in the Department of Engineering Management & Technology at UTC. He obtained his PhD 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 PhD 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.

Lead PI:
"Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation"

Dr. Robert Webster

Dr. Robert Webster was an Associate Professor in Mechanical Engineering at UTC. He received his BS (1986) from Auburn University, and MS (1994) and PhD (2001) from Mississippi State University, all in Aerospace Engineering. He was at UTC for 16 years; most of that time was as SimCenter research faculty. His research was primarily in computational simulation of aerospace propulsion systems, applied to the aerothermodynamics of fans and compressors within air-breathing engines. He was lead or co-author of numerous conference publications presented at the AIAA SciTech and Propulsion & Energy Forums. He was an inaugural member of the AIAA Gas Turbine Engine Technical Committee and is currently a member of the AIAA Inlets, Nozzles, and Propulsion Systems Integration Technical Committee. Dr. Webster left UTC in January 2019 and is currently a systems engineer with Northrop Grumman Mission Systems in Huntsville, AL. Please refer to Dr. Webster's biosketch in **Appendix A** for more information.

Co-PI:
"Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems"

Dr. Lakmali Weerasena

Dr. Lakmali Weerasena is an Assistant Professor in the Department of Mathematics. She received her M.Sc. in Mathematics in 2009 and her PhD in Mathematics (Operations Research Concentration) in 2019 at the Clemson University. Her research interests include developing approximation algorithms for optimization problems, multi-objective combinatorial optimization, numerical optimization and applications of optimization, mathematical modeling, statistical approach for optimization problems. Her applications include developing optimization models and algorithms for conservation biology and engineering problems. She is a published author in the area. She is also actively engaged in outreach activities conducted by the department. Please refer to Dr. Weerasena's biosketch in **Appendix A** for more information.

Co-Investigator:

"Estimating the Youden Index Under the Multivariate Roc Curve in The Presence of Missing Values of Mass Diseased and Healthy Biomarker Data"

Weidong Wu

Dr. Weidong Wu is an Associate Professor and Graduate Program Coordinator for the Department of Civil & Chemical Engineering in University of Tennessee at Chattanooga. He received his PhD in Civil Engineering at the University of Mississippi. His research interests include innovative technologies application in civil engineering, computational mechanics, and multiscale materials modeling. His research work has appeared in various leading engineering journals including *Composites B*, *Computational Material Science*, *Journal of ASTM International*, *IEEE Xplore*, and symposium proceedings. He is PI and Co-PI of multiple TDOT and NSF grants. His current research focuses on using AI/Deep Learning technology in infrastructure and building structure health monitoring. Please refer to Dr. Wu's biosketch in **Appendix A** for more information.

Lead PI:

"Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems"

FY2019 STUDENTS

Project Title: 3D Drone Delivery Transportation Problem
Lead PI: Ignatius Fomunung

Students Impacted:

Mr. Babatunde Atolagbe, the graduate student on this project, has gained a high-level knowledge of programming, software development, geometric modeling, and documentation skills. The grid generation code developed in this project has a significant work load that is usually defined as a separate master's thesis in the field of computational engineering and computer science. He successfully mastered how to implement all algorithms and integrate them into some applications in the field of civil engineering. He also used the codes to generate a grid for a part of the Tennessee River used in Dr. Bathi's (co-PI) research.

Project Title: Analyzing Bioimage Big Data with Deep Learning Neural Networks
Lead PI: Hong Qin

Students Impacted:

Mehran Ghafari: A PhD student whose stipend and tuition was supported by this grant from July 2018 to June 2019. He led the task on Fast-RCNN for microscopic image analysis, and the comparison of CNN and CapsuleNet.

Justin Clark, MS graduate student. He performed the initial comparison of CNN and CapsulNet.

Caleb Powell, MS graduate student. He is the connection between computer science students and biology students. He led the development of herbarium automation pipeline.

Dakila Ledesma, Undergraduate researcher. He led the color chip task.

William Baker, Undergraduate researcher. He participated in plant image CNN task.

Andrew Watson, Undergraduate researcher. He participated in developing Python code for image partitions.
Haobo Guo, June's salary was supported for Dr. Guo to help Mr. Ghafari to revise manuscript, including revise algorithms, figures, methods and materials, results and discussions.

Project Title: Estimating the Youden Index Under the Multivariate Roc Curve in The Presence of Missing Values of Mass Diseased and Healthy Biomarker Data
Lead PI: Sumith Gunasekera

Students Impacted:

Aruna Saram, Doctoral student in Computational Science with concentration in Computational and Applied Mathematics, July 2020, had greater opportunities to learn and explore new statistical and mathematical languages such as Python, R, SAS, MatLab, etc.

Oluwakorede Ajumobi, Master's student, Mathematics with concentration in Statistics, May 2019, had greater opportunities to learn and explore new statistical and mathematical languages such as Python, R, SAS, MatLab, etc.

Alissa Coleman, baccalaureate student, Engineering with concentration in Electrical Engineering, December 2020, had greater opportunities to learn and explore new statistical and mathematical languages such as Python, R, SAS, MatLab, etc.

Project Title: Improving Post-stroke Management Efficiency and Patient Outcomes through Analytics
Lead PI: Mina Sartipi

Students Impacted:

Jin Cho, PhD student in the Computer Science and Engineering Department

Kristal Price, Physical Therapy Department

Rebecca Salstrand, Physical Therapy Department

Project Title: Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels
Lead PI: Soubantika Palchoudhury

Students Impacted:

Eric Pritchard, 1st year MS Chemical Engineering candidate – Full tuition, graduate assistantship, and health insurance of the student was supported from the grant. The student was mentored in CFD modeling and was involved in constructing the computational flow model for the nanodrugs.

Armel Boutchuen, 2nd year MS Chemical Engineering candidate – The student was involved in synthesis and characterization of the nanodrug and the hydrogel channels, flow studies of the nanodrug through the hydrogel channels, writing the journal article, and presenting the results at conferences.

Ketan Patel, Chemical Engineering undergraduate student, graduated in May 2019 – Hourly support for the student was provided through this grant. The student was involved in synthesis and material characterization of the hydrogel channels, writing the journal article, and conference presentations.

Olivia George, Chemical Engineering undergraduate student, graduated in May 2019 – The student was involved in cutting-edge experimental research related to this project and conference presentations. She won the NSF Graduate Student Fellowship and completed the Honors Thesis under the PI's supervision.

Yasmin Foster, Chemical Engineering undergraduate student, graduated in May 2019 – She was involved in hydrogel synthesis and flow experiments as well as helping with the journal article.

Dell Zimmerman, Chemical Engineering undergraduate student, junior – The student was extensively involved in the experimental section of the project, presenting at different internal conferences, report writing, and outreach activities at local schools to promote science, technology, engineering, and mathematics. Won the best poster award at the UTC Technology Symposium.

Gitapun Jur, Chemical Engineering undergraduate student, sophomore – Involved in experimental research related to the project and presentation at internal conferences.

Project Title: Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications
Lead PI: Daniel Loveless

Students Impacted:

Ryan Boggs, MS student in Electrical Engineering. Ryan presented his CEACSE-funded work on photonic device modeling and simulation at 2 conferences, one of which resulted in a published proceeding. Ryan graduated in August 2019.

Ahmed Ibrahim, MS student in Electrical Engineering. Ahmed submitted 1 paper to a refereed conference regarding this effort (still pending). He was the recipient of a UTC SEARCH award to supplement his efforts and to acquire additional hardware for demonstration of his Wi-Fi transceiver at the focus of his work. Ahmed plans to graduate in December 2019.

Artem Malashiy, Undergraduate Research Assistant throughout this CEACSE effort. Artem graduated in May 2019.

Bharat Patel, MS student in Electrical Engineering. Bharat presented his CEACSE-funded work on the IRES technique at 2 conferences and submitted 1 paper to a refereed journal regarding this effort (still pending). Bharat plans to graduate in December 2019.

Project Title: Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems
Lead PI: Weidong Wu

Students Impacted:

Shuvashis Roy, MS in Civil Engineering, expected graduation December 2019. Developed part of graduate thesis report. Exposed and trained in the area of ENM pollution, analysis, and data analysis.

Syed Tareq, MS in Civil Engineering, expected graduation December 2019. Developed part of graduate thesis report. Exposed and trained in the area of ENM pollution, analysis, and data analysis.

Patrick Craig, BS in Civil Engineering, expected graduation December 2020. Exposed and trained in the area of ENM pollution, analysis, and data analysis.

Jenk Parker, BS in Civil Engineering, expected graduation May 2020. Exposed and trained in the area of ENM pollution, analysis, and data analysis.

Haiven Camenisch, BS in Chemical Engineering, Junior. Exposed and trained in the area of ENM pollution, analysis, and data analysis.

Project Title: Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations
Lead PI: Lingju Kong

Students Impacted:

Christopher Michael Corley, a PhD student, was supported by this grant.

Project Title: STC3: A Smart Trust-based Connected Autonomous Collaborative Communities
Lead PI: Farah Kandah

Students Impacted:

Steven Schmitt, MS computer science (Dec 2018) involved in different aspects of the project, where they learned different research skills including, coding, debugging, algorithm design, and writing technical reports and papers.

Dylan Brownell, BS computer science (May 2019) involved in different aspects of the project, where they learned different research skills including, coding, debugging, algorithm design, and writing technical reports and papers.

Peyton Ball, BS computer science (May 2019) involved in different aspects of the project, where they learned different research skills including, coding, debugging, algorithm design, and writing technical reports and papers.

Brennan Huber, MS computer science (Present) involved in different aspects of the project, where they learned different research skills including, coding, debugging, algorithm design, and writing technical reports and papers.

Project Title: Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design
Lead PI: Vahid Disfani

Students Impacted:

Saroj Khanal, Saroj was a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He was involved in all tasks of the project. He learned data processing and data visualization techniques. He learned development of optimization problem models and their solution using optimization solvers in MATLAB. He graduated in summer. The optimization knowledge he earned through this project enabled him to peruse his next career with the microgrid optimization group at National Renewable Energy Laboratory (NREL).

Shailesh Wasti, Shailesh is a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He was involved in all tasks of the project. He learned data processing and data visualization techniques. He learned development of optimization problem models and their solution using optimization solvers in MATLAB. He still has one year to graduate. His future research will be directly related to the topic of this project.

Farog Ahmed, Farog is a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He was involved in Tasks 2 and 3 of the project. He learned data processing and data visualization techniques. He learned development of optimization problem models and their solution using optimization solvers in MATLAB. He still has one year to graduate. His future research will most likely be different from the topic of this project.

Sakineh Khalili, MBA student and research assistant for Dr. Ahmadi in the college of business. She was involved in Task 1 of the project. She learned data processing and data visualization techniques using Tableau. She learned how to perform statistical analysis on the EV demand empirical data to develop. The knowledge she obtained through this project enabled her to be hired as a business data analyst by the Covenant Transport, Inc. Sakineh still has one year left before she graduates.

Ahmad Eltayeb, Ahmed helped the project by developing time-domain simulation platforms in MATLAB Simulink. He learned how to apply optimization techniques in these platforms. His research enabled him to be hired by Mesa Associates, Inc. in Chattanooga.

Project Title: Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities
Lead PI: Kidambi Sreenivas

Students Impacted:

Juan Hernandez, Juan was an undergraduate student who was working for the PIs when the project started. His experience with Pointwise (honed through this project) came in handy for his Honors thesis which required him to generate meshes for nozzle geometries. Juan graduated with a BS in Mechanical Engineering in Spring 2019 and currently has a year-long internship with National Boiler Service, an industrial boiler design and refurbishment company based out of Dalton, GA.

Hannah Gifford, Hannah was also an undergraduate student who was working for the PIs when the project started. She graduated in Spring 2019 with a BS in Mechanical Engineering and a minor in Computer Science. Her background made her uniquely suited for this project and the experience with Pointwise and Python helped her earn a summer internship with the Helios group (helicopter simulation software) at NASA Ames Research Center. She may consider going to graduate school, but at this time, her plans are to obtain a job in industry.

Aaron Crawford, Aaron was a junior when the project started and had some background with ArcGIS when he started. He was utilized to process the building footprints. Additionally, he learnt Pointwise and Python through this project. This combination helped him earn an internship with the Helios group at NASA Ames Research Center. He will be returning in Fall to complete his senior year and is on track to graduate in Spring 2020. He will also be utilizing the skills he has developed through this project and his internship in order to finish his Honors thesis. He is hoping to pursue graduate studies once he has graduated with the BS in Mechanical Engineering.

Project Title: Using Computational Tools to Understand the Fundamental Rules of Life
Lead PI: Hope Klug

Students Impacted:

Richard Blanton, MS in Environmental Science in progress: Rick participated in all GIS components of the project.

Zachary McCoy, MS in Environmental Science in progress, plans to apply to PhD program once MS is complete: Zachary participated in ecological network research related to life history.

Jacob Burleson, BS in Geology in progress: Jacob participated in all GIS components of the project.

Braley Gentry, BS in Biology in progress: Braley participated in all aspects of the ecological network research.

Chelsea Langley, BS in Psychology 2018: Chelsea participated in ecological simulations related to parental care and mating strategies.

Zachary Sheckley, BS in Biology 2018**:** Zachary participated in data collection and ecological simulations related to fish life history, mating, and parental care.

Thomas Wiegand, BS in Biology in progress: Thomas participated in all aspects of the ecological network research.

Project Title: Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation
Lead PI: Jin Wang

Students Impacted:

Conrad Ratchford, PhD student in the Department of Mathematics. With the support from this project, he has generated solid results in mathematical and computational modeling of waterborne infectious diseases and is making good progress toward his PhD.

Erick Rojas, graduate student in the Department of Chemical Engineering. With the support from this project, he has performed important experimental studies and successfully completed his MS degree in June 2019.

Chayu Yang, PhD student in the Department of Mathematics, also impacted by project.

Eric Siv, undergraduate student in the Department of Biology and Environmental Science, also impacted by the project.

Project Title: Kinetic and computational elucidation of nucleic acid aptameric binding mechanism for enhanced molecular targeting

Lead PI: Michael Danquah

Students Impacted:

Mikayla Hawkins, undergraduate student Chemical Engineering. The mini-CEACSE funding and supported the student and promoted research training and experiential learning. The student gained hands-on research experience in structural modeling and molecular dynamics simulation with applications in apta-targeting of cancer receptors. The student presented a poster at 2019 Research Dialogue and CECS Tech Symposium.

Alexis Hartwig, undergraduate student, Chemical Engineering. The mini-CEACSE funding and supported the student and promoted research training and experiential learning. The student gained hands-on research experience in structural modeling and molecular dynamics simulation with applications in apta-targeting of cancer receptors. The student presented a poster at 2019 Research Dialogues and CECS Tech Symposium.

Project Title: Exploiting Alkynyl Titanocenes for Carbon-Carbon Bond Formation
Lead PI: Jared A. Pienkos

Students Impacted:

Lara Partridge, who received fall 2018 and spring 2019 funding for research experience, is a biochemistry major, and will attend medical school in the Fall of 2019.

Logan Jaques received fall 2018 funding for research and continued research for credit during the spring of 2019 and the summer of 2019 (funded by the chemistry department).

Logan is a rising junior and a chemistry major, he plans to study natural products chemistry following his graduation.

Carson Gilbert received fall 2018 funding for research and continued research for credit during the spring of 2019 and the summer of 2019 (funded by the chemistry department). Carson is a rising junior and biochemistry major who plans on joining the military following college.

Hailey Beaver received spring 2019 funding for research. Hailey plans on attending medical school.

Sarah McDarmont, who received spring 2019 research for credit and summer 2019 funding and is a rising junior who plans on attending graduate school.

Anastasia McConkey, who received summer 2019 funding, is a rising senior who plans on attending pharmacy school.

Tiffany Truong, who received summer 2019 funding, is a rising sophomore who plans on attending graduate school.

Zach Moser, who received summer 2019 funding, is a rising senior who plans on getting a job in the chemical industry.

Project Title: ULIRES: A Unified Live Incident Response System for Energy Delivery Systems"

Lead PI: Mengjun Xie

Students Impacted:

Ruipeng Zhang, PhD student in Computer Science. He has been working on this project for the past year. With the research funds from CEACSE, he was able to continue his study and pursue a PhD degree. He has acquired valuable hands-on research experience and knowledge of digital forensics and research project management through this project.

PROGRAM OVERVIEW & ACCOMPLISHMENTS

The value proposition for multidisciplinary and interdisciplinary research, education, and training in the rapidly advancing field of Computational Science and Engineering (CSE) has grown stronger since the start of CEACSE in 2005. Today, modeling, simulation, High-Performance Computing (HPC), High-Throughput Computing (HTC), and so-called "Big Data" and "Machine Learning" 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 significant return on investment by attracting new extramural funding.

FY2019 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). Strong collaborative interactions with UTC Deans and faculty underpin this program.

Dr. Skjellum has led the CEACSE efforts for approximately 26 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/HPT, and data science ground the strategy of advancing and diversifying the participation of UTC faculty and students in CEACSE projects in FY2019 and beyond.

The FY2019 portfolio of CEACSE projects accomplished a number of foundational advancements in R&D for cyber-physical systems, computational biology, and mathematics. Importantly, we were able to fund appropriate research projects in all of the identified research foci (highlighted below), with Aerospace/Defense and Smart Cities decreasing in percentage as other areas of inquiry have grown. The spin-off of the Center for Urban Informatics and Progress (CUIP), on July 1, 2018, heralded the success of a swim lane in becoming an independent research center as well.

Health and Biological Systems R&D is now growing rapidly and with great promise as noted in last year's report: its swim lane now has the most self-identified participants. Energy and Environment and Cyber Security & Cyber-physical Systems also continue to gain momentum. These areas have been well represented in new external research awards received by CEACSE-funded projects.

Even with the investments described in FY2018 for basic compute and storage, it was essential to further modernize the locally available computing and storage infrastructure at UTC. To that end, we made an approximately $400,000 investment in FY2019. This has primarily been in the area of High-Throughput Computing (HTC), which has enabled performance-oriented cloud computing to become accessible to UTC scientists and engineers pursuing modeling, simulation, data analytics, and machine learning in pursuit of their intellectual inquiries. This backend computing, powered by GPUs in some cases, enables scientists to explore greater problem solving without engaging the full power of massively parallel clusters (HPC). We have leveraged these investments with two successful NSF CC* Award wins in cluster computing and networking during the fiscal year, totaling approximately $900,000 of new federal awards to complement the CEACSE investment in HTC and connect campus users with the CEACSE resources at high

performance. Additionally, some of our CEACSE awardees from FY2019 have won R&D funding from NSF for work that leverages the CEACSE support received.

Two major accomplishments from FY2019 were the expansion of the CEACSE program to include a Faculty Initiation and Career Opportunity competition, with awards of up to $15,000, up to $25,000 with $5,000 matching. We had four awardees for each competition.

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. CEACSE plays a central role in capability and program development potentially impacting all Colleges at UTC. These strategies intersect with problems of global, national, and regional importance in six primary focus areas:

- Aerospace & Defense Simulation
- Cybersecurity & Cyber-physical Systems
- Energy & the Environment
- Health & Biological Systems
- High-Performance Computing
- With Smart Cities & Urban Dynamics funded primarily if there is strong alignment with the new CUIP center, and not already supported by this center's programs.

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 these focus areas are reviewed for technical merit and strategic alignment, including scrutiny of a plan to develop extramural funding. Beginning in FY2019, further important advances in proposal content, process, selection, and peer review were applied across the CEACSE program. All CEACSE proposals already underwent rigorous external review in prior years, now including double-blind review as of FY2020 awardees. 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. We have observed successful transition of CEACSE awardees to extramural funding during FY2019 as well, and CEACSE awardees are significant producers of external research proposals.

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.

As of 2020, the "Digital Twins" swim lane will become active. It provides a means to encapsulate R&D in modeling and simulation together with data fusion, analytics, and machine learning. This area of scientific and engineering pursuit is expected to be the key means by which modeling and simulation is delivered in real-time, for training, and for engineering analyses in many fields over the next two decades and beyond. This effort launches in complement to a new NSF award that will support workshops at UTC and Tennessee Technological University on the pedagogy of Digital Twins, with the goal of workforce development for this class of applied modeling and simulation workforce.

Overview of FY2019 Projects

In FY2019, the core CEACSE competition 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. Faculty Initiation and Opportunity Awards included four faculty members on four new projects.

The funded projects key to the six CEACSE/SimCenter priority areas: 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.

Core Competition

Project Title: Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation
Lead PI: Jin Wang
Co-PI(s): David Giles, Bradley Harris

Summary:
The main objective of this project is to establish a new, experimentally guided, computational framework to investigate the fundamental pathogen dynamics associated with waterborne diseases. The project represents a pilot effort in the quantitative and systematic study of the pathogen dynamics associated with waterborne infections, integrating mathematical, computational and biological approaches. In particular, the computational framework bridges the pathogen dynamics at vastly different time scales in order to improve our current understanding of the exact roles played by the pathogens in shaping the complex epidemics and endemics of waterborne infections.

The project not only builds a solid knowledge base for understanding waterborne infection dynamics, but also provides useful public health guidelines for disease management and policy development. Meanwhile, the project enhances interdisciplinary curriculum development concerning the quantitative study of epidemiology and microbiology. Mentoring and training activities are centered on the graduate students involved in this project. Particularly, the project enhances the newly established PhD concentration in Computational and Applied Mathematics at UTC. The project results in a number of journal publications, conference presentations, and external grant applications. Overall, the project contributes to the Capacity Building and Strategic Excellence in computational science at UTC and supports the mission of the SimCenter.

Project Title: Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications
Lead PI: Daniel Loveless
Co-PI(s): Don Reising
Other Personnel: Bharat Patel, Ahmed Ibrahim, Ryan Boggs, Artem Malashiy

Summary:
This program addressed several critical challenges posed by the increasing interest of using commercial off-the-shelf (COTS) hardware in space systems. The specific objectives were to (1)

investigate radiation failure mechanisms in emerging electronics technologies and (2) explore techniques for improving the fault tolerance of COTS circuits and systems deployed in space environments. These objectives were accomplished through a comprehensive, coordinated modeling and experimental methodology using in situ measurement coupled with intelligent control using machine learning. Such an approach will close the gap in performance between strategic hardware and commercial hardware by leveraging the performance advantages offered by the latest technology nodes without the overhead required of radiation-hardening-by-design. This effort resulted in 4 international conference presentations, 1 journal publication, 1 additional journal submission, 1 additional conference submission, 1 grant funded by the Office of Naval Research, and 2 additional grant proposal submissions to the National Science Foundation (NSF) and National Reconnaissance Office (NRO). The project provided partial support to 3 graduate students and 1 undergraduate student.

This project supported the mission of the SimCenter by directly contributing both the Aerospace/Defense and Energy/Environment swimlanes. This research combined electronics device research with advanced computational modeling and simulation, resulting in an innovative concept with the potential to create a paradigm shift in electronics reliability assessment in space, defense, and commercial sectors.

Project Title: Analyzing bioimage big data with deep learning neural networks.
Lead PI: Hong Qin
Co-PI(s): Joey Shaw, Yu Liang

Summary:
We developed various machine learning methods, including deep learning methods, to extrapolate meaningful biological information or meta-information from bioimage data sets. For the yeast time-lapse microscopic images, we compared convolutional neural networks with capsule networks, and found that the two methods have complementary performances. For the plant image data sets, we experimented with various architectures of convolutional networks to compare flowering versus non-flowering images and extract the color pixel panel for color correction.

Project Title: Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations
Lead PI: Lingju Kong
Co-PI(s): John R. Graef, Andrew Ledoan

Summary:
By drawing an analogy to the spreading dynamics of an infectious disease, we derive a fractional-order susceptible-infected-removed (SIR) model to examine the user adoption and abandonment of online social networks (OSNs), where adoption is analogous to infection and abandonment is analogous to recovery. We modify the traditional SIR model with demography, so that both infectious and noninfectious abandonment dynamics are incorporated into our model. More precisely, we consider two types of abandonments: infectious abandonment resulting from interactions between an abandoned and an adopted member and noninfectious abandonment without being influenced by an abandoned member. In addition, we study the existence and uniqueness of nonnegative solutions of the model, as well as the existence and stability of its equilibria. Our stability results show that the infectious abandonment dynamics does not contribute to the stability of the user-free and user-prevailing equilibria and that it only affects the location of the endemic equilibrium. The Jacobian matrix technique and the Lyapunov function

method are used to show the stability of the equilibria. Numerical simulations are provided to verify these theoretical results.

This project demonstrates how to improve on previous studies by utilizing the theory of fractional calculus to supply a new and efficient approach for studying OSN dynamics. This project creates a framework in which the graduate student can more clearly understand the conceptual structure in which theoretical and numerical methods function as an aid to learning. Moreover, the research findings in this project may attract the interest of incumbent and emerging network providers and their stakeholders. This project aligns with the mission of the SimCenter of advancing modeling- and simulation-based science at UTC.

Project Title: Using Computational Tools to Understand the Fundamental Rules of Life
Lead PI: Hope Klug
Co-PI(s): Jennifer Boyd, Azad Hossain, Hong Qin

Summary:
We used big datasets, geographic information system (GIS) approaches, and computational tools to (1) develop and analyze biological networks (i.e., relationships) of interest across species and geospatial scales, (2) assess network robustness and stability, and (3) identify the key interactions that influence the genotype-phenotype map. We focused on three timely biological questions of interest: (1) What biological rules govern the expression of genes and how robust are gene/protein interactions? (2) Does phenotypic plasticity influence the relative abundance of species and what environmental factors and interactions influence plasticity? (3) What ecological, evolutionary, and behavioral interactions determine mating strategy and parental investment mode?

Our findings suggest that (1) aging increases noise in gene networks, but long-lived cells and calorie restriction are able to significantly suppress noise in the gene networks, which can be thought of as a “general rule” on aging regulation; (2) a variety of factors, including ecology, evolution, and development, likely influence whether species are rare versus common; and (3) a range of ecological factors, costs and benefits of alternative behaviors, and life-history traits can interact to influence the evolution of mating strategies and parental care. Additionally, our GIS research revealed that (4) imperiled plant and fish species are not randomly located across space but instead are potentially distributed non-randomly in relation to changes in environmental factors.

The proposed research involved substantial student training, led to (and will continue to lead to) multiple high-impact publications and papers in preparation, and contributed to or will serve as the foundation for multiple grant proposals.

Project Title: Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems
Lead PI: Weidong Wu
Co-PI(s): Jejal Reddy Bathi

Summary:
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 using fate simulation models. There are no reliable fate models that currently available have proven the ability to simulate ENM behavior in the environment. As part of our research, we reviewed generally used water quality simulation models and their applicability to model ENMs in surface waters. Since the literature pertaining to type and quantity of ENM in the surface water

environment is limited, as the first phase of the proposed research, a systematic evaluation of available literature to identify prominent ENMs and their physical, chemical, and biological properties that are important in pollutants fate assessment was conducted. Second and third phases of the proposed research were to develop a calibrated EFDC model for river hydraulics and ENM fate simulation.

The research findings provided a demonstrated case study to present at the local national conference. The research findings were published as conference proceedings and as a book chapter in addition to several student posters and podium presentations at the technical conferences. The research findings also aided in the development of external funding proposal.

Project Title: Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels
Lead PI: Soubantika Palchoudhury
Co-PI(s): Abdollah Arabshahi

Summary:
One of the major limitations for implementing new nanoparticle-based drugs as novel solutions to some of the biggest medical challenges of the day is the low translation rate from preclinical studies to the clinical stage. There is a need for a more reliable preclinical tool, which can predict the relevant behavior (e.g., flow regime and flow velocity) of new nanodrugs within the human body. In this project we constructed a combined experimental and computational strategy as a new preclinical model to assess the flow and deposition of nanodrugs in physiologically relevant environments. This project facilitated research training and support for graduate and undergraduate students. It has led to six publications, five external proposal submissions, four external conference presentations, and one undergraduate Honors thesis. Community engagement through outreach activities at local schools and UTC events for promoting science and technology fields was also supported through this grant. This work directly aligns with the SimCenter's mission to advance and support innovations in health and biomedical fields through cutting-edge interdisciplinary research.

Project Title: 3D Drone Delivery Transportation Problem
Lead PI: Ignatius Fomunung
Co-PI(s): Arash Ghasemi, Joseph Owino, Mbakisya Onyango
Other Personnel: Babatunde Atolagbe

Summary:
We have developed infrastructure theory and software required for urban modeling. These include codes for automatically generating surface mesh for a given urban system that accurately models the buildings using an unstructured watertight surface mesh. We have also investigated routing and energy reduction strategies.

The primary purpose of these codes was to be used in determination of drone routing; however, the results can be applied to a wide range of problems in the area of urban modeling, including evacuation planning, hazardous plume and inverse problems, routing for minimizing fuel efficiency, etc. Currently, the team has developed two internal presentations, one presentation in China, and an article that has been submitted to the Transportation Research Board annual conference for presentation and publication. One graduate student was supported during this research, and he has completed his master's thesis in this field.

Project Title: Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design
Lead PI: Vahid Disfani
Co-PI(s): Mo Ahmadi, Mina Sartipi

Summary:
Growing interest in electric vehicles (EV) has established an inevitable demand for installation and smart operation of electric vehicle supply equipment (EVSE), also known as charging stations. Maximizing utilization of EVSEs is a sustained challenge in EVSE operations despite the emergence of EV station locators, e.g. PlugShare.com and ChargeHub.com, providing EVSEs' availability and price information which are partial, real-time, and snapshot datasets. More significantly, the missing key element in this platform is the lack of communication from demand side or EVs. These challenges often leave EVs—sometimes desperate for charging—disconnected while several EVSEs are available nearby.

Although the corresponding literature includes a significant number of works in the optimal charging process and schedule of EVs and their technical and economic effects on power system and electricity markets, none of them has studied how to match the EVs and EVSEs to maximize the social welfare of both parties. These social benefits will at least include higher utilization of EVSEs as well as time savings and less costs for EV owners. The fact that the literature is silent on this issue and that the EVs are becoming the main core of the near future road transportation platform make this period of time a critical and favorable moment to investigate reliable solutions to optimally match EVs and EVSEs for charging process.

Project Title: Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities
Lead PI: Kidambi Sreenivas
Co-PI(s): Abdollah Arabshahi, Ethan Hereth

Summary:
The objective of this project was to reconstitute the capability at the SimCenter in order to carry out city-scale simulations. The first step in this process was the development of an efficient workflow that could be used to process the Geographical Information Systems (GIS) data into usable geometry. Once this process is completed, meshes can be generated and simulations carried out.

The biggest challenge when it comes to any simulation is that of geometry. Having a clean, high-quality geometry results in a good quality mesh, which in turn enables the simulation to complete successfully. The building footprints of various cities are available through their respective GIS departments. This data is in the form of ShapeFiles and needs to be manipulated and exported into a format that is conducive to building a mesh. This was carried out using a combination of ArcGIS (commercial GIS software), various libraries in Python, and some custom code. This workflow enabled the efficient processing of GIS information into a water-tight solid model that was then used within Pointwise (commercial grid generation software) in order to generate the final mesh.

This project provided three undergraduate students with research experience in utilizing ArcGIS, Python, and Pointwise. This resulted in two of the students obtaining summer internships at NASA Ames Research Center. The third student obtained a year-long internship with an industrial boiler design and installation company in the Dalton area. Additionally, this project resulted in research collaborations between various faculty at UTC and produced five related proposals.

Project Title: Estimating the Youden Index Under the Multivariate Roc Curve in The Presence of Missing Values of Mass Diseased and Healthy Biomarker Data
Lead PI: Sumith Gunasekera
Co-PI(s): Lakmali Weerasena, Hong Qin
Other Personnel: Aruna Saram

Summary:
Multivariate Youden index (J) and its corresponding optimal cut-point (c^*) have become the most effective and efficient approach in multi-biomarker mass data analysis to distinguish diseased from the healthy in this digitized era. However, the existing statistical classical approach does not produce exact solutions in the presence of nuisance parameters and missing and group mass data. This proposed novel high-performing computational-based generalized Variable Method is an alternative procedure to produce exact statistical inferential results for J and c^* in the presence of such constraints.

In compliance with the mission of the Center of Excellence in Applied Computational Science and Engineering (CEACSE) at The University of Tennessee at Chattanooga (UTC) that is to establish and expand a cohesive multidisciplinary effort in applied computational science and engineering leveraging across UTC and produce sustained growth in research funding, excellence in integrated education and research, and to increase national and international stature and competitiveness in Tennessee, we built a high-performance computational resource as part of a web services framework called GeneralizedMultivariateYouden (GMY) that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers in the presence of missing and grouped, or pooled, data. Codes of GMY were written in Python for the multivariate-BioMarker (mBM) data.

Project Title: Improving Post-stroke Management Efficiency and Patient Outcomes through Analytics
Lead PI: Mina Sartipi
Co-PI(s): Nancy Fell

Summary:
For the main task of the CEACSE project (TN Higher Education Commission), we primarily focus on developing a data-driven precision healthcare ecosystem for management for stroke. The goal of this task is to utilize machine learning/deep learning framework for data processing, modeling, and decision support in healthcare management. The development of predictive models for stroke management will allow us to help health outcomes and increase stroke patients' quality of life by providing a sophisticated and detailed analysis of post-stroke assessment. Furthermore, it will help reduce the cost of stroke management, and reduce caregiver's burden.

In order to achieve this goal, we use the medical data provided by the TN Department of Health (TDoH) and the Centers for Medicare and Medicaid Services (CMS), which includes patient demographic information, and clinical information such as primary diagnosis codes (ICD9), procedure codes, source of admission, and insurance status. We propose a machine learning/deep learning-based methods (Logistic Regression, Random Forest, AdaBoost, and Multi-layer Perceptron) to extract patient information and discover underlying patterns from the data. All of the methods mentioned above were implemented using scikit-learn and Keras, a deep learning library written in Python.

Using the simplest model (i.e., logistic regression model), we were able to build an easy-to-use predictive tool for predicting hospital discharge disposition status of stroke patients.

Faculty Initiation and Opportunity Award Competition

Project Title: Kinetic and computational elucidation of nucleic acid aptameric binding mechanism for enhanced molecular targeting
Lead PI: Michael Danquah

Summary:
This project studied the fundamental molecular mechanisms responsible for the functionality of DNA aptamers as biomolecular probes for diagnostics and targeted delivery applications. Specifically, the project investigated the biophysical binding process and structural transformations of DNA aptamers via molecular dynamics modeling and simulation using a thrombin-binding aptamer (TBA) as a model. This molecular-level modeling and simulation offered real-time analysis and visualization of TBA-thrombin binding process and was significant in determining relevant TBA conformations and conditions for enhanced thrombin binding. We successfully modeled the TBA-thrombin structures for molecular dynamics (MD) simulations to determine the molecular features of the binding process and stability.

The mini-CEACSE FY19 funding served as important seed funding to build research capacity in the area of aptamer-target binding for theranostic applications. Specifically, it has contributed in developing the initial research work that will form the foundation of building a stronger research program through the pursuance of external research funding, expanding research facilities, recruiting graduate and undergraduate research students, increasing research publications and developing intellectual properties, engaging with the community and expanding collaborative supports. The mini-CEACSE FY19 funding resulted in the following achievements (i) 3 external research proposals submitted to National Science Foundation, St. Baldrick Foundation, and Prevent Cancer Foundation; (ii) recruitment of 2 undergraduate students to work on the project – promoting experiential learning via research training, (iii) participation in 2019 UTC research dialogue and CECS Tech Symposium, (iv) 3 research manuscripts; all under review with Chemical Engineering Journal, Scientific Reports and Biotechnology Advances, and (v) strengthening collaborations with internal and external partners. These outcomes directly advance the mission of SimCenter particularly in the area of using computational engineering tools for biomedical applications in disease diagnosis, pathogen detection, and targeted delivery of cancer.

Project Title: Development and Application of Bioinformatics Pipelines and Theoretical Models to Predict Microbiome Biodiversity in Response to Environmental Stressors
Lead PI: Francesca Leasi

Summary:
The main goal of the project was to build bioinformatics pipelines and environmental models to assess and predict biodiversity of microscopic organisms under environmental stressors. I am a junior faculty who started a tenure-track position in Fall 2018. In line with the main missions of the SimCenter, the mini-CEACSE grant allowed me to immediately establish collaborations with faculty at UTC. In this context, I have submitted an interdisciplinary grant proposal to the CEACSE program with other faculty at UTC from different departments. The proposal has been funded to promote outreach activities by organizing the First Southeastern Computational School. The workshop was very successful and attracted 25 among students and faculty from UTC and other 14 different institutions. I also used the grant to support one undergraduate and one graduate student in computer science. This grant allowed me to enhance knowledge in computational biology at UTC. Attending such a workshop allowed me to improve skills in

computational biology and achieve familiarity with the main tools. In this context, I have computationally analyzed data and obtained results that were presented at an international conference. The grant also allowed me to get preliminary data that are being used to prepare an extra-mural fund grant proposal.

Project Title: Exploiting Alkynyl Titanocenes for Carbon-Carbon Bond Formation
Lead PI: Jared A. Pienkos

Summary:
Our project focused on the design of ligands, or compounds that bind to metals, which are typically utilized to modulate the reactivity of catalysts. We were able to successfully design, synthesize, and characterize one of these said ligands. During the course of this study, eight undergraduate students were trained in synthetic chemistry, and basic programs were utilized with computational chemistry. Five of these students will present work at SERMACS, a regional chemistry conference. Two of these students provided outreach activities to a group of home-schooled students and to a local private high school. We believe these activities are in line with the SimCenter's mission to integrate education and research, as multiple students and members of the community were impacted by this project.

Project Title: ULIRES: A Unified Live Incident Response System for Energy Delivery Systems
Lead PI: Mengjun Xie
Other Personnel: Ruipeng Zhang

Summary:
As an indispensable component of a comprehensive cybersecurity solution to energy delivery systems, direct and efficient incident response has not received sufficient research and development efforts and therefore becomes a weak link. This project addresses the challenge of lacking in-depth research on effective technologies for forensics and incident response for energy delivery systems by developing ULIRES, a unified live incident response system. The core objective of this project is to develop a suite of novel, reliable, and efficient techniques that can be used to perform effective live incident response and to understand and model attack behavior for energy delivery systems. The research contributions include the design and development of new techniques for live system monitoring and data acquisition on an Android-powered mobile platform and IoT devices, as well as new knowledge of IoT incident response. The outcome of this research will result in transformative techniques that can lead to stronger security protection to the national energy infrastructure. This project will produce publications and software to the research communities and industry. This project has involved graduate students in the research, which advances the excellence in integrated and multidisciplinary research and education and aligns with the mission of SimCenter.

Distinguished Lecture Series Grants

Requesting Faculty: Jejal Reddy Bathi
Invited Speaker: Dr. Venkataramana Gadhamshetty, South Dakota School of Mines & Technology
Lecture Title: 2D Material and Bioelectrochemistry Approaches for Emerging Environmental and Energy Applications

Summary of Qualifications:
Dr. Venkata Gadhamshetty is an established researcher in microbial electrochemistry and environmental engineering. He has versatile research and teaching experiences from multiple institutions, including Rensselaer Polytechnic Institute, Florida Gulf Coast University, Air Force Research Laboratory, and Dupont. He is currently a Board Certified Environmental Engineer, a professional Engineer from the state of New York, Associate Professor at the South Dakota School of Mines and Technology (SD Mines), and water pollution engineering committee chair of Environmental and Water Resource Institute (EWRI) at ASCE. Dr. Gadhamshetty's team is currently interrogating research questions at the interface of surface engineering, 2D materials, electrochemistry, system biology, and big data tools, with a primary goal of understanding rules of life of biofilms that grow on technologically relevant materials (conducting electrodes and metals) modified with nano-meter coatings. His research currently uses unique environments of the Sanford Underground Research Laboratory and Yellowstone National Park to understand intricate interactions between biofilms and the surfaces they inhabit in deep, extreme, and thermal environments, respectively.

Requesting Faculty: Farah Kandah
Invited Speaker: Dr. Mohammed Akour, Yarmouk University
Lecture Title: Smart Applications in University, Agriculture, and City

Summary of Qualifications/Lecture:
Dr. Mohammed Akour is an Associate Professor in the Department of Software Engineering at Yarmouk University (YU). He got his Bachelor's (2006) and Master's (2008) degrees from YU in Computer Information Systems, with Honors. He joined YU as a Lecturer in August 2008. In August 2009, he left YU to pursue his PhD in Software Engineering at North Dakota State University (NDSU). He joined YU again in April 2013. He serves as organizer, co-chair, and publicity chair for several IEEE conferences and serves on editorial review boards for more than 10 ISI indexed prestigious journals. He is a member of the International Association of Engineers (IAENG). At YU, Dr. Akour has also served as Head of Accreditation and Quality Assurance and Director of the Computer and Information Center. Dr. Akour is currently the Vice Dean of Student Affairs.

Dr. Akour's seminar will cover a brief description of smart applications in University, Agriculture, and City contexts. He will tackle the essence behind the smartness in our lives through his experience in this field and concentrate on a new idea for building a smart irrigation system, with Yarmouk University as a pilot study. He will specifically address the aim of the project and the main instruments required to accomplish it.

Requesting Faculty: Francesca Leasi
Invited Speaker: Dr. Christof Meile, University of Georgia–Athens
Lecture Title: Reactive transport modeling in aquatic environments: Putting bugs in the code

Summary of Qualifications:
Dr. Cranos Williams is an associate professor in the electrical and computer engineering (ECE) department at North Carolina State University. He founded the EnBiSys (Engineering Computational Methodologies for Multi-hierarchical Biological Systems) Research Laboratory. The EnBiSys Research Laboratory focuses on developing computational and analytical solutions for modeling and understanding the combinatorial interactions of biomolecular, physiological, and structural processes that impact plant growth, development, and adaptation. The goal of his lab is to conduct translatable research that is capable of addressing problems associated with efficient biofuel production from non-food sources, improving plant defenses to pathogens and abiotic stresses, and increasing food security in the presence of an increasing population and sporadic fluctuations in climate. As part of research conducted in his lab, he has received funding ($12.5M Total; $1.3M directly to him) as a PI or Co-PI from eight research grants that were awarded by federal agencies such as the National Science Foundation, the Department of Energy, and the National Institute of Health and through grants supported by private local companies.

Requesting Faculty: Hong Qin
Invited Speaker: Dr. Cranos Williams, North Carolina State University
Lecture Title: Dynamic modeling of the iron deficiency modulated transcriptome response in *Arabidopsis thaliana* roots

Summary of Qualifications:
Dr. Cranos Williams is an associate professor in the electrical and computer engineering (ECE) department at North Carolina State University. He founded the EnBiSys (Engineering Computational Methodologies for Multi-hierarchical Biological Systems) Research Laboratory. The EnBiSys Research Laboratory focuses on developing computational and analytical solutions for modeling and understanding the combinatorial interactions of biomolecular, physiological, and structural processes that impact plant growth, development, and adaptation. The goal of his lab is to conduct translatable research that is capable of addressing problems associated with efficient biofuel production from non-food sources, improving plant defenses to pathogens and abiotic stresses, and increasing food security in the presence of an increasing population and sporadic fluctuations in climate. As part of research conducted in his lab, he has received funding ($12.5M Total; $1.3M directly to him) as a PI or Co-PI from eight research grants that were awarded by federal agencies such as the National Science Foundation, the Department of Energy, and the National Institute of Health and through grants supported by private local companies.

Requesting Faculty: Francesca Leasi
Invited Speaker: Christof Meile
Lecture Title: 2D Material and Bioelectrochemistry Approaches for Emerging Environmental and Energy Applications

Summary of Qualifications/Lecture:
Dr. Christof Meile is a Professor in the Department of Marine Sciences at the University of Georgia. He completed his undergraduate at the Swiss Federal Institute of Technology in Zurich

(ETHZ) in Environmental Sciences, received a MS in Earth and Atmospheric Sciences from the Georgia Institute of Technology (USA) and earned a PhD from the Faculty of Earth Science at Utrecht University (The Netherlands). His interests lie in understanding and modeling biogeochemical cycling in near-surface environments, ranging from deep-sea sediments and seeps to coastal settings and tropical soils.

Reactive transport modeling of microbially mediated processes contributes to an improved understanding of elemental cycling in Earth near-surface environments. I will discuss how microbial processes have been represented in reactive transport models, show applications from marine sediments and present recent advances in modeling approaches. An additional challenge is discrepancy between the scale of reactive transport models and the local environment of microbes that determines their metabolism. I will discuss recent work studying methane dynamics and anaerobic methane oxidation in cold seep environments both at the micro- and the macroscale.

FY2019 Budget

NEW CORE AWARDS FY2019				
Investigators	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Jin Wang, David Giles, and Bradley Harris	Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation	Health & Biological Systems	$99,992.00	$83.865.21
Daniel Loveless and Don Reising	Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications	Aerospace & Defense / Energy & Environment	$99,876.00	$92,609.68
Hong Qin, Joey Shaw, Yu Liang, and Craig Tanis	Analyzing Bioimage Big Data with Deep Learning Neural Networks	Health & Biological Systems	$99,957.00	$91,445.70
Lingju Kong, John R. Graef, and Andrew Ledoan	Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations	Health & Biological Systems	$96,380.00	$96,380.46
Hope Klug, Jennifer Boyd, Azad Hossain, and Hong Qin	Using Computational Tools to Understand the Fundamental Rules of Life	Health & Biological Systems	$99,040.00	$95,856.10
Weidong Wu, Jejal Reddy Bathi	Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems	Energy & Environment	$96,217.00	$90,929.88
Soubantika Palchoudhury and Abdollah Arabshahi	Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels	Health & Biological Systems	$100,000	$99,061.92
Ignatius Fomunung, Arash Ghasemi, Joseph Owino, and Mbakisya Onyango	3D Drone Delivery Transportation Problem	Energy & Environment	$67,568.00	$61,795.47
Vahid Disfani, Mo Ahmadi, and Mina Sartipi	Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design	Energy & Environment	$96,114.00	$92,347.19
Kidambi Sreenivas,	Urban Resilience in the Post-Evacuation Age:	Energy & Environment	$77,464.00	$65,526.68

Abdollah Arabshahi, and Ethan Hereth	Combining CFD and ABM for Megacities			
Sumith Gunasekera, Lakmali Weerasena, and Hong Qin	Estimating the Youden Index Under the Multivariate Roc Curve in the Presence of Missing Values of Mass Diseased and Healthy Biomarker Data	Health & Biological Systems	$97,901.00	$95,416.16
Mina Sartipi and Nancy Fell	Improving Post-stroke Management Efficiency and Patient Outcomes through Analytics	Health & Biological Systems	$99,221.00	$98,665.46
Farah Kandah and Mina Sartipi	STC3: A Smart Trust-based Connected Autonomous Collaborative Communities	Cybersecurity and Cyber-Physical Systems	$80,000.00	$63,346.35
NEW INITIATION/OPPORTUNITY AWARDS FY2019				
Investigators	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Michael Danquah	Kinetic and computational elucidation of nucleic acid aptameric binding mechanism for enhanced molecular targeting	Health & Biological Systems	$14,976.00	$11,925.45
Francesca Leasi	Development and application of bioinformatics pipelines and theoretical models to predict microbiome biodiversity in response to environmental stressors	Energy and the Environment & Health and Biosystems	$19,905.00	$19,905.00
Jared A. Pienkos	Exploiting Alkynyl Titanocenes for Carbon-Carbon Bond Formation	Energy and the Environment	$14,999.00	$14,641.92
Mengjun Xie	ULIRES: A Unified Live Incident Response System for Energy Delivery Systems	Cybersecurity and Cyber-physical Systems	$20,000.00	$20,000.00

DISTINGUISHED LECTURE SERIES AWARDS FY2019				
UTC Faculty	**Invited Lecturer**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Jejal Bathi	Dr. Venkataramana Gadhamshetty	Energy and Environment	$1,450	$1,450
Farah Kandah	Dr. Mohammed Akour	Cybersecurity and Cyber-physical Systems	$2,500	$2,500
Francesca Leasi	Dr. Christof Meile	Health and Biological Systems	$1,450	$1,450
Hong Qin	Dr. Cranos Williams	Health and Biological Systems	$1,800	$1,800

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution: UT Chattanooga

Center: Center of Excellence is Applied Computational Science & Engineering

	FY 2018-19 Actual			FY 2019-20 Proposed			FY 2020-21 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries									
Faculty	$155,220	$288,265	**$443,485**	$204,900	$395,100	**$600,000**	$204,900	$395,100	**$600,000**
Other Professional	$4,625	$8,590	**$13,215**	$36,000	$64,000	**$100,000**	$34,150	$65,850	**$100,000**
Clerical/ Supporting	$4,968	$9,226	**$14,195**	$18,000	$32,000	**$50,000**	$10,245	$19,755	**$30,000**
Assistantships	$120,163	$223,159	**$343,322**	$54,000	$96,000	**$150,000**	$34,150	$65,850	**$100,000**
Total Salaries	**$284,976**	**$529,241**	**$814,217**	**$312,900**	**$587,100**	**$900,000**	**$283,445**	**$546,555**	**$830,000**
Longevity	$345	$641	**$987**	$2,880	$5,120	**$8,000**	$1,708	$3,292	**$5,000**
Fringe Benefits	$36,136	$67,110	**$103,247**	$71,715	$138,285	**$210,000**	$71,715	$138,285	**$210,000**
Total Personnel	**$321,112**	**$596,351**	**$918,450**	**$384,615**	**$725,385**	**$1,118,000**	**$355,160**	**$684,840**	**$1,045,000**
Non-Personnel									
Travel	$15,765	$29,277	**$45,042**	$18,000	$32,000	**$50,000**	$13,660	$26,340	**$40,000**
Software	$3,109	$5,775	**$8,884**	$4,200	$7,800	**$12,000**	$5,122	$9,878	**$15,000**
Books & Journals	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Other Supplies	$19,096	$35,465	**$54,561**	$21,000	$39,000	**$60,000**	$9,100	$16,250	**$25,350**
Equipment	$99,342	$184,493	**$283,835**	$5,250	$9,750	**$15,000**	$5,250	$9,750	**$15,000**
Maintenance	$19,540	$36,289	**$55,829**	$0	$0	**$0**	$0	$0	**$0**
Scholarships	$8,379	$15,560	**$23,939**	$10,500	$19,500	**$30,000**	$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**
Print	$256	$475	**$731**	$0	$0	**$0**	$0	$0	**$0**
Other Personal Services	$14,679	$27,262	**$41,941**	$2,100	$3,900	**$6,000**	$8,750	$16,250	**$25,000**
Rentals	$57	$106	**$163**	$5,600	$10,400	**$16,000**	$0	$0	**$0**
Group Arranged Events	$743	$1,381	**$2,124**	$242	$451	**$693**	$133	$248	**$381**
Special Commercial Services	$1,801	$3,344	**$5,145**	$3,500	$6,500	**$10,000**	$4,217	$7,813	**$12,030**
Membership	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Student Fees	$54,656	$101,504	**$156,161**	$0	$0	**$0**	$0	$0	**$0**
Total Non-Personnel	**$237,424**	**$440,931**	**$678,355**	**$70,392**	**$129,301**	**$199,693**	**$67,232**	**$125,529**	**$192,761**
GRAND TOTAL	**$558,536**	**$1,037,282**	**$1,596,805**	**$455,007**	**$854,686**	**$1,317,693**	**$422,392**	**$810,369**	**$1,237,761**
Revenue									
New State Appropriation		$781,596	**$781,596**		$792,534	**$792,534**		$832,161	**$832,161**
Carryover State Appropriation		$332,533	**$332,533**		$76,847	**$76,847**			**$0**
New Matching Funds	$405,600		**$405,600**	$405,600		**$405,600**	$405,600		**$405,600**
Carryover from Previous Matching Funds	$195,648		**$195,648**	$42,712		**$42,712**			**$0**
Total Revenue	**$601,248**	**$1,114,129**	**$1,715,377**	**$448,312**	**$869,381**	**$1,317,693**	**$405,600**	**$832,161**	**$1,237,761**

Schedule 7

FY2019 PUBLICATIONS AND PRESENTATIONS (of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings

Jin Wang, "Modeling and simulating cholera dynamics, Computational and Applied Mathematics Colloquium," Pennsylvania State University, October 2018.

Jin Wang, "Analyzing the within-host dynamics of cholera, Special Session on Differential Equations in Mathematical Biology," AMS Spring Southeastern Sectional Meeting, Auburn, AL, March 2019.

Eric Siv, Erick Rojas, **David Giles**, **Bradley Harris**, and **Jin Wang**, "An Examination of Allee effects in Vibrio cholera," The 80th Annual Meeting of ASB, Memphis, TN, April 2019.

Chayu Yang and **Jin Wang**, "Modeling the within-host dynamics of cholera, UTC Research Dialogues," April 2019.

Jin Wang, "Mathematical modeling of infectious diseases, Biology Seminar," University of Tennessee at Chattanooga, April 2019.

Erick Rojas, "Determination of Allee Effects and Virulence in Vibrio Cholerae," MS (in Engineering) thesis defense, June 2019.

Jin Wang, "Infectious disease models and differential equations," Department of Mathematics, University of Tennessee at Chattanooga, June 2019.

A. Ibrahim, W. Mitchell, K. Hall, **D. Reising**, and **D. Loveless**, "The Effects of a Phase Modulated Clock and Temperature on RF-DNA Fingerprints in IEEE 802.11a Wi-Fi Signals," *in review*, Radio and Wireless Symposium (RWS2020), Jan. 2020.

T. D. Loveless, B. Patel, **D. Reising**, and L. W. Massengill, "Spectrographic Analysis of Single Event Transients in RF Circuits," 2019 IEEE Nuclear and Space Radiation Effects Conference (NSREC*)*, paper B-2, San Antonio, TX, July 2019.

R. C. Boggs, E. Richards, L. W. Massengill, and **T**. **D. Loveless**, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," 2019 IEEE Southeast Conference, Apr. 2019.

R. C. Boggs, E. Richards, L. W. Massengill, and **T. D. Loveless**, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," 2019 Single Event Effects Symposium, May 2019.

B. Patel, **D. Reising**, L. W. Massengill, and **T. D. Loveless**, "Single Event Transient Analysis with Ionizing Radiation Effects Spectroscopy (IRES)," 2019 Single Event Effects Symposium, May 2019.

Ahmed Ibrahim, "Unlocking the Secrets of RF-DNA Fingerprinting," presented at the 2019 Research Dialogues, UTC, Apr. 2019. [student]

Bharat Patel, "Single Event Transient Analysis with Ionizing Radiation Effects Spectroscopy," presented at the 2019 Research Dialogues, UTC, Apr. 2019. [student]

Artem Malashiy, "The UTChattSat Small-Satellite Platform," presented at the 2019 Research Dialogues, UTC, Apr. 2019. [student]

R. Boggs, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," 2019 UTC Research Dialogues. [student]

R. Boggs, “An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices,” 2019 CECS Technology Symposium. [student]

A. Ibrahim, “Unlocking the Secrets of RF-DNA Fingerprinting,” 2019 CECS Technology Symposium. [student]

Powell, C. Oral presentation. “Born Digital, enabling a field-database workflow for herbaria.” 34th Annual Meeting of the Society for the Preservation of Natural History Collections. Field Museum, Chicago. May 25–30, 2019. [student]

Powell, C. Oral presentation. “Born digital, addressing the challenges of a field-to-database workflow for collections based research.” 80th Annual meeting of the Association of the Southeastern Biologists (ASB). Memphis. April 3–6, 2019. [student]

Ledesma, Oral presentation, “Using convolutional neural networks to classify the reproductive state of digitized herbarium specimens.” 80th Annual meeting of the Association of the Southeastern Biologists (ASB). Memphis. April 3–6, 2019. [student]

Ghafari, Poster presentation, UAB [student]

Ghafari, Poster presentation, Memphis. [student]

Guo, H. Poster presentation, UAB.

Ghafari, Poster presentation, Finding inner modeler. [student]

Guo, H. Poster presentation, Finding inner modeler.

Guo, H. UTK 21st Century Cures meeting.

Ghafari, UTC 21st Century Cures meeting. [student]

Ghafari, 3 minute elevator competition. [student]

Ghafari, poster presentation. UTC Research Day, Technical symposium. [student]

Dax, Technique symposium. [student]

Clark, Justin, Technique symposium. [student]

Guo, H. UTC Research Day.

Guo, H. Technique symposium.

L. Kong. AMS Special Session on Fractional, Stochastic, and Hybrid Dynamical Systems with Applications, Joint Mathematics Meetings, Baltimore, MD, January 16–19, 2019.

M. Corley. NSF-CBMS Conference: “L-functions and Multiplicative Number Theory,” May 20–24, 2019, at University of Mississippi. [student]

L. Kong, **J. R. Graef**, and **A. Ledoan**. “Modeling online social network dynamics using fractional-order epidemiological models.” UTC Research Dialogues.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H**, **Boyd J**. “Visualizing connectivity of ecological and evolutionary concepts with network analysis: an exploration of research on species rarity.” Poster. World Congress on Undergraduate Research (WorldCUR); Carl Von Ossietzky Universität, Oldenburg, Germany, May 2019.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H**, **Boyd J**. “Visualizing connectivity of ecological and evolutionary concepts with network analysis: an exploration of research on species rarity.” Poster. National Conference on Undergraduate Research (NCUR); Kennesaw State University, Kennesaw, GA, April 2019.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H**, **Boyd J.** "Visualizing connectivity of ecological and evolutionary concepts with network analysis: an exploration of research on species rarity." Poster. SoCon Undergraduate Research Forum (SURF); Wofford College, Spartanburg, SC, November 2018.

Klug, H. & Stone, L. "The role of chance in determining mating success" (Poster Presentation) Evolution 2018; Montpellier, August 2018.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H, Boyd J.** "Visualizing connectivity of ecological and evolutionary concepts with network analysis." Poster. Ecological Society of America, New Orleans, LA, August 2018.

Hossain, **A**., Burleson, J., **Klug, H., Boyd, J**., and Blanton, R. "Developing a Geographic Information System to map and analyze the conservation status of conifers, ferns, and flowering plants in the United States," 12th Southeastern Forestry and Natural Resource management GIS Conference, December 9–10, 2019, Athens, GA.

Guo, H, **Qin**, **H**. "Network-based association study of protein sets and applications in gene ontology enrichment analysis." UTC Research Dialogues.

McCoy, Z. "Using big data to address questions in life-history evolution." UTC Research Dialogues. [student]

Bathi., **J**.**R**., Clark., S., Gadhamshetty., V., Tareq., S., Roy., S. "Characterization of Polycyclic Aromatic Hydrocarbons and Engineered Nanomaterial in Surface Water Environment" ASCE Environmental and Water Resource Institute (EWRI) Conference, Pittsburgh May 2019. (Conference proceedings)

Bathi., **J**.**R**., Geza., S., Gadhamshetty., V. "Emerging Water Infrastructure: Occurrence and Treatability aspects of Engineered Nanomaterial" ASCE Environmental and Water Resource Institute (EWRI) Conference, Pittsburgh May 2019. (Podium presentation)

Roy., S., **Bathi**., **J**. **R**. "Decision Supporting Hydrodynamic Modeling of TN River," 28th Tennessee Water Resources Symposium, Montgomery Bell State Park, Burns, TN, August 06, 2019 (Poster)

Bathi., **J.R**., Clark., S., Tareq., S., Roy., S., Gadhamshetty., V. "Characterization of Polycyclic Aromatic Hydrocarbons and Engineered Nanomaterial in Surface Water Environment" ASCE Environmental and Water Resource Institute (EWRI) Conference, Pittsburgh May 2019. (Podium presentation)

Roy., S., **Bathi**., **J**. **R**. "Decision Supporting Hydrodynamic Modeling of TN River," 28th Tennessee Water Resources Symposium, Montgomery Bell State Park, Burns, TN, April 10-12, 2019 (Poster).

Tareq., S., **Bathi., J. R.** "Characterization of Nano Contamination: Challenges and Findings" University of Tennessee Research Dialogues, April 10, 2019 (Poster)

Bathi, J.R., Tareq., S., Palchoudary., S. "Detection and Treatability of Nanomaterial in Surface Waters," 28th Tennessee Water Resources Symposium, Montgomery Bell State Park, Burns, TN, April 10-12, 2019 (Podium Presentation)

Roy., S., **Bathi., J. R**. "Decision Supporting Hydrodynamic Modeling of TN River," University of Tennessee Research Dialogues, April 10, 2019 (Presentation)

Tareq., S., **Bathi., J. R**. "Characterization of Nano Contamination: Challenges and Findings" University of Tennessee Research Dialogues, April 10, 2019 (Poster)

Craig., P., Sawyer., S., **Bathi., J.R**. “Nanomaterial: Characterization and Treatment in Urban Stormwater Runoff,” University of Tennessee Research Dialogues, April 10, 2019 (Poster)

Palchoudhury, S.; **Arabshahi**, **A**.; Gharge, U.; Boutchuen, A. Foster, Y. Zimmerman, D. Alresheedi, H. “A new class of integrated chalcogenide nanocrystals and thin films for solar cell applications” 2019 TMS Conference, Mar 2019 (Oral Talk).

Palchoudhury, **S**., **Arabshahi**, **A**., Foster, Y., Gharge, U., Boutchuen, A. “Synthesis and size analysis of DNA conjugated bio-hybrid nanostructures” Materials Research Society Fall Conference, Nov 2018 (Poster).

George, O., **Palchoudhury, S**. “Effect of different ligands on water-soluble iron oxide nanoparticle size” AIChE Conference, Oct 2018 (Poster).

George, O., Mcmahon, W., **Arabshahi**, **A**., **Palchoudhury**, **S**. “Synthesis and transport of Pt-iron oxide nanodrugs” National Council of Undergraduate Research Conference, Apr 2018.

B**.** Atolagbe, **A**. **Ghasemi**, **I**. **Fomunung**, **M**. **Onyango** and **J. Owino**, “Towards Energy-Optimized Deployment of Unmanned Aerial Vehicles for Civil Applications: A Novel Conceptual Framework,” Submitted to Transportation Research Board on Submission Date: July 31st, 2019

B**.** Atolagbe, **A. Ghasemi**, **I. Fomunung**, **M**. **Onyango** and **J**. **Owino,** “Three-dimensional mesh representation of urban environment based on OpenStreetMap (OSM) data,” 2019 ReSEARCH dialogue, University of Tennessee and Chattanooga.

Atolagbe, A. **Ghasemi**, **I**. **Fomunung**, **M**. **Onyango** and **J**. **Owino**, “City Modeling based on actual OSM data,” 2019 Technology Symposium, Chattanooga TN.

Vahid Disfani, “Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design,” 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019.

Sakineh Khalili, Timothy Barczak, Chanda Kelly, **Vahid Disfani**, **Mo Ahmadi**, “Growth Modeling of Electric Vehicle Charging Demand in Chattanooga - A Case Study,” 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019.

Sakineh Khalili, Timothy Barczak, Chanda Kelly, **Vahid Disfani**, **Mo Ahmadi**, “Growth Modeling of Electric Vehicle Charging Demand in Chattanooga - A Case Study,” 2019 UTC CECS Technology Symposium, Chattanooga, TN, April 2019.

Saroj Khanal, Sakineh Khalili, Farog Mohamed, Shailesh Wasti, **Vahid Disfani**, **Mo Ahmadi**, **Mina Sartipi**, “Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design,” 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019.

Saroj Khanal, Sakineh Khalili, Farog Mohamed, Shailesh Wasti, **Vahid Disfani**, **Mo Ahmadi**, **Mina Sartipi**, “Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design” 2019 UTC CECS Technology Symposium, Chattanooga, TN, April 2019.

K. **Sreenivas**. Research Dialogues 2019

Gunasekera, S. 8th International Conference on Biostatistics & Bioinformatics (CB&B) sponsored by the Conference Series under the Theme “Exploring Advances in Biostatistics & Bioinformatics” from September 1617, 2019 in San Francisco, CA, USA.

Gunasekera, S. “Estimating the Youden index under the multivariate ROC curve in the presence of missing values of mass diseased- and healthy-biomarker data,” 2019

Gunasekera, S. 7th International Conference on Biostatistics & Bioinformatics (CB&B) sponsored by the Conference Series under the Theme “Exploring Advances in Biostatistics & Bioinformatics” held September 26–27, 2018 at Holiday Inn Chicago O ‘Hare, Chicago, Illinois, USA.

Gunasekera, S. “Exact inference for the Youden index to discriminate individuals using two-parameter exponentially distributed pooled samples,” 2018.

Gunasekera, S. Joint Statistical Meetings (JSM) sponsored jointly by the American Statistical Association (ASA), International Biometric Society (IBS) Eastern North American Region (ENAR), and Western North American Region (WNAR), Institute of Mathematical Statistics (IMS), Statistical Society of Canada (SSC), International Chinese Statistical Association (ICSA), International Indian Statistical Association (IISA), International Society for Bayesian Analysis (ISBA), Korean International Statistical Association (KISA), and Royal Statistical Society (RSS) under the Theme “Statistics: Making an Impact” from July 27–August 01, 2019 in Denver, Colorado, USA.

Gunasekera, S. “Bayesian inference for the common-location parameter of several shifted exponential populations,” 2019.

Wijekularathna, D. and **Gunasekera**, **S**. “On Performing Generalized Inferences for the Burr XII Reliability Function based on Progressively Censored Data.” 2019.

Gunasekera, **S**., **Weerasena**, **L**., Saram, A. Ajomobi. “Statistical Exploration of Stochastic Differential Equation Models used in the Stochastic Dynamics of Biological Systems” Statistical Algorithms & Computer Programs, 2019.

Gunasekera, **S**. “Exact inference for the Youden index to discriminate individuals using two

parameter exponentially distributed pooled samples.” Podium Talk, 2018.

Gunasekera, **S**. “Mathematics and Statistics: Who is the Winner?” Faculty Elevator Pitch, 2019

M. **Sartipi**. UTC Research Dialogues

F. **Kandah**. IEEE iThings

F. **Kandah**. IEEE HPEC

F. **Kandah**. IEEE CCWC

F. **Kandah**. IEEE ICCE

F. **Kandah**. Research Dialogue

F. **Kandah**. SimCenter retreat

Michael K Danquah, Haobo Guo, Mikayla Hawkins, Alexis Hartwig. “Engineering aptamer-mediated targeted cancer therapy.” Poster presentations. 2019 UTC Research Dialogue and CECS Tech Symposium.

Leasi et al. “Integrating biodiversity surveys of meiofauna and microbiome for ecosystem biomonitoring.” International Meiofauna Conference. Evora (Portugal) July 7-12, 2019.

Sarah McDarmont. “Synthesis of multi-metallic acetylide compounds of d10 transition metal.” SERMACS, 2019.

Logan Jaques. “Synthesis of tBpyPt(C22py)2 and its interactions with Cu(I) and Pd(II) metals.” SERMACS, 2019.

Zach Moser, Tiffany Truong, and Anastasia McConkey. “Synthetic strategies for generating 4-ethynyl-2,3,5,6-tetrafluoropyridine.” SERMACS, 2019.

J. Pienkos. Research Dialogues.

M. Xie. ReSEARCH Dialogues, 2019.

M. **Xie**. CECS Technology Symposium, 2019.

Software

I. **Fomunung**. Building Footprint Capture: A C89 code to obtain the building footprints inside a bounding box specified by GPS coordinates.

I. Fomunung. LiDAR converter: A C89 code to process USGS topography data.

I. Fomunung. Auto City Generator: A set of MATLAB functions to create watertight unstructured surface mesh for an urban landscape.

V. Disfani, M. Ahmadi, and **M. Sartipi.** The package includes data cleaning, optimization platform, Monte-Carlo simulation, and post analysis sections to run the entire tasks of the projects.

Refereed Publications

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

E. Eckels, S. Jin, **A. Ledoan**, and B. Tobin, “Lower bounds for the L^1 norm of exponential sums,” to be submitted.

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

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

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

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

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

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

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

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

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

Palchoudhury, **S**., Jungjohann**,** K**., Weerasena**, **L**., **Arabshahi**, **A**., Gharge, U., Albattah, A., Miller, J., Patel, K., Holler, R., “Enhanced legume root growth with pre-soaking in α-Fe_2O_3 nanoparticle fertilizer.” *RSC Adv*, 2018. 8:p. 24075. Impact Factor: 3.049

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

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

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

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

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

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

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

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

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

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

Ruipeng Zhang and **Mengjun Xie**. “GRRAndroid: Remote Live Forensics for Android at Scale.” Under preparation for submission.

EXTERNAL FUNDING

Hope Klug, Lead PI

Co-PI(s): Jennifer Boyd, Azad Hossain, Hong Qin
Project Title: "Using Computational Tools to Understand the Fundamental Rules of Life"

Proposal Submissions

1. National Science Foundation, Division of Information & Intelligent Systems: Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education ($549,888) (Funded research team: P: H Qin; Co-PIs A Hossain, J Boyd, H Klug, and J Shaw; Note: Per the PO's request that some personnel be removed because there were an unusually large number of co-PIs on the overall collaborative grant, Boyd and Klug volunteered to be removed from this grant effective September 2018)
2. National Science Foundation, CC* Networking Infrastructure: Advancing high-speed networking at UTC for research and education. ($499,663 requested) (PI: F Kandah; Co-PIs: H Klug, A Skjellum, M Sartipi, D Gendron)
3. National Science Foundation, Major Research Instrumentation: Acquisition: A Research-as-a-Service (RaaS)-based Private Cloud for Innovative Science and Engineering ($921,109 requested) (PI: A Skjellum; Co-PIs: F Kandah, M Sartipi, H Klug, E Panagiotou)
4. NIH, R21, Using Permutations of Gene/Protein Networks for Pairwise Association Analysis of Genomic Data. Submitted in November 2018. Declined. PI: Qin.

Contracts/Awards Received

1. National Science Foundation, Division of Information & Intelligent Systems: Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education ($549,888) (Funded research team: P: H Qin; Co-PIs A Hossain, J Boyd, H Klug, and J Shaw; Note: Per the PO's request that some personnel be removed because there were an unusually large number of co-PIs on the overall collaborative grant, Boyd and Klug volunteered to be removed from this grant effective September 2018)
2. National Science Foundation, CC* Networking Infrastructure: Advancing high-speed networking at UTC for research and education. ($499,663 funded) (PI: F Kandah; Co-PIs: H Klug, A Skjellum, M Sartipi, D Gendron)

Sponsored Program Capacity Building Activities

1. All PIs actively wrote, managed, and planned for future grants during the award period.

Daniel Loveless, Lead PI

Co-PI(s): Don Reising
Project Title: "Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications"

Proposal Submissions

1.National Science Foundation (NSF), CAREER, July 2018 (Not Funded)
Title: "CAREER: Fundamental Reliability Analysis of Si FinFETs and Nanowires through

Ionizing Radiation Effects Spectroscopy"
Amount: "$500,000"

2.Office of Naval Research (ONR), submitted Jan 2019 (Funded)
Title: "RHBD Through IRES and Intelligent Control"
Amount: "$199,771"

3.National Reconnaissance Office (NRO), Director's Innovation Initiative (DII), July 2019 (Under Review)
Title: "In-Situ Radiation Detection Using Existing On-Board Spacecraft Hardware"
Amount: $250,805

Contracts/Awards Received

1. Office of Naval Research (ONR), submitted Jan 2019 (Funded)
Title: "RHBD Through IRES and Intelligent Control"
Amount: "$199,771"

Sponsored Program Capacity Building Activities

1. NSF-REU Panel

Soubantika Palchoudhury, Lead PI

Co-PI(s): Abdollah Arabshahi
Project Title: "Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels"

Proposal Submissions

1. "A New Library of Cadmium-Free Multinary Chalcogenide Nanocrystals for Engineered Quantum Dot Light Emitting Device", PI: S. Palchoudhury, $508,356, NSF Career, Engineering Directorate, Division of Electrical, Communications and Cyber Systems, submitted: July 2019
2. "Evaluation of an Integrated Nanophotocatalytic and Bioremediation Approach to Stormwater Management using Rain Barrels as a Green Infrastructure", PI: S. Palchoudhury, co-PI: M. Danquah, $199,891, Tennessee Department of Transportation, submitted: April 2019
3. "A New Class of Enhanced Sensors with Iron Oxide-Protein Cage Nano-architectures for Petroleum Tracers", PI: S. Palchoudhury, $55,000, ACS Petroleum Fund, submitted: March 2019
4. "Characterization of a new class of integrated copper chalcogenide nanocrystals", PI: S. Palchoudhury, User research proposal for Center for Nanophase Materials Sciences, Oak Ridge National Laboratories, submitted: March 2019
5. "Coupled Computational and Experimental Approach to Understand the Flow of Nanodrugs", PI: S. Palchoudhury, co-PI: A. Arabshahi, $300,763, NSF Engineering Directorate, Division of Chemical, Bioengineering, Environmental and Transport Systems, submitted: January 2019

Contracts/Awards Received

1. Center for Integrated Nanotechnologies User Proposal Award, Sandia National Lab, "Understanding the Effect of Engineered Nanoparticles in Agriculture", 2017-2018, PI: S. Palchoudhury, Agreement for electron microscopy use
2. Center for Integrated Nanotechnologies User Proposal Award, Sandia National Lab, "Developing a New Family of Wurtzite $CuZn_2ASe_4$ (A= Al, Ga, In) Nanocrystals for Solar Cell Applications", PI: S. Palchoudhury, Agreement for electron microscopy use

3. NSF REU-site: “Engaging Undergraduates in Interdisciplinary Computing in Biology (ICompBio)”, PI: H. Qin, co-PI: S. Palchoudhury, 2019-2022, $359,484
4. UTC Faculty Development Grant 2019 for summer research, “Experimental and numerical simulation of nanoparticle flow through hydrogel channels”, PI: S. Palchoudhury, co-PI: A. Arabshahi, $1,500. (Internal Funding)

Sponsored Program Capacity Building Activities

1. Attended NSF 2019 Biology REU Site Workshop, April 4–6 2019, Arlington, VA.
2. Attended on-campus NSF Career workshop activities.

Hong Qin, Lead PI

Co-PI(s): Joey Shaw, Yu Liang, Craig Tanis
Project Title: "Analyzing Bioimage Big Data with Deep Learning Neural Networks “

Proposal Submissions

1. Qin (PI), Dumas, Shaw, NSF CUE: Collaborative Research: Bridging diversity and curriculum gaps in computing through pedagogical innovation and cross-discipline education. $114K. Submitted on May 9, 2019.
2. Qin (Senior personnel), NSF Data Science Corps, Collaborative Research: Building Diverse Workforce in Data Science Through Integrating Real-world Projects into Curricula. ~$360K. PI Yang. Submitted in February 2019.
3. Qin (PI), NIH R21, Using permutation of gene/protein networks for pairwise association analysis of genomic data. ~$300K, Submitted on Nov 16, 2018.
4. Liang (PI), Dalei Wu (Computer Science & Engineering), Cuilan Gao (Mathematics), Hemant Jain (Management), and Dr. Anthony Skjellum (SimCenter) have requested $723,641 from the National Science Foundation for the project entitled, “HDR DSC: Collaborative Research: ADACE – Anthropocentric Data Analytics for Community Enrichment.” Submitted in February 2019.

Contracts/Awards Received

1. Qin (PI), Liang (coPI), Shaw (coPI), Hossain (coPI), NSF IIS, “Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education”, $1M, ~$550K to UTC, Oct. 2018 – Sep. 2021, awarded.
2. Qin (PI), Palchoudhury (coPI), NSF DBI “REU Site: ICompBio – Engaging Undergraduates in Interdisciplinary Computing for Biological Research” ~ $359K. Submitted in August 2018, awarded.

Sponsored Program Capacity Building Activities

1. PI Qin led postdoc Haobo Guo and graduate student Mehran Ghafari attended the NIH 21st Century Cures Conference at UTK in March 2019.
2. PI Qin led postdoc Haobo Guo and graduate student Mehran Ghafari attended the NSF workshop, Finding Your Inner Modeler at UAB in June 2019.

Kidambi Sreenivas, Lead PI

Co-PI(s): Abdollah Arabshahi, Ethan Hereth,
Project Title: "Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities"

Proposal Submissions

1. Discovering Potential Reasons for Pedestrian Accidents, $205,152, TDOT, 02/06/2019
2. Preliminary Proposal: Smart Real-Time Control (SmaRT Control) for Accurate Monitoring and Management of Urban Stormwater Runoff, USGS, 02/15/2019
3. Exploring Transit Innovation in Chattanooga, $70,000, Lyndhurst Foundation, 07/12/2019
4. Data in GigCity: A Unified and Comprehensive Platform for Education and Research on Data Science and Engineering to Improve Accessibility in an Urban Environment, $2,912,891, NSF, 02/06/2019
5. Preliminary Proposal: NSF Engineering Research Center for Intelligent Connected Infrastructures in Sustainable Urban Environments (CONNECT), NSF, 01/16/2019

Contracts/Awards Received

1. CC* Compute: A Cost-Effective, 2,048 Core InfiniBand Cluster at UTC for Campus Research and Education, $392,235, NSF, 10/01/2019 – 09/30/2021
2. Heterogeneous HPC for High-Order Stabilized Finite-elements on Moving and Deforming Domains, SAIC Inc., $400,000, 09/01/2017 – 08/31/2019
3. Mesh curving for higher order applications, Pointwise Inc., $100,000, 06/01/2018 – 05/31/2020

Sponsored Program Capacity-Building Activities

1. Ongoing monthly calls with Dr. Mike List, Air Force Research Laboratory, Wright Patterson Air Force Base, Ohio to discuss progress on research related to FUNSAFE.
2. Regular meetings with Dr. Steve Karman, Pointwise Inc., at the SimCenter to apprise him of the status on current funded research.
3. Met with NSF-Ignite program officers (on campus) to apprise them of current research areas related to urban issues.
4. Attended UTC's 1st Research Summit as the Department of Mechanical Engineering representative.

Jin Wang, Lead PI

Co-PI(s): David Giles and Bradley Harris
Project Title: "Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation"

Proposal Submissions

1. NSF REU program: proposal submitted in August 2018 (PI: A. Ledoan; co-PI: J. Wang)
2. NSF Math Biology program: proposal submitted in September 2018 (PI: J. Wang)
3. NIH R15 program: proposal submitted in October 2018 (PI: J. Wang; co-Is: Giles & Harris)
4. NSF Computational Math program: submitted in December 2018 (PI: E. Panagiotou; co-PI: J. Wang)

Contracts/Awards Received

1. REU Site: Research Training for Undergraduates in Mathematical Analysis with Applications in Allied Fields. PI: Andrew Ledoan; Co-PI: Jin Wang. National Science Foundation (REU program), 2019–2022, $282,659.
2. Computational Methods for Measuring Topological Entanglement in Polymers. PI: Eleni Panagiotou; Co-PI: Jin Wang. National Science Foundation (Computational Math program), 2019–2022, $125,000.
3. Experimentally Guided Modeling and Simulation for Cholera Dynamics. PI: Jin Wang; Co-Is: David Giles and Brad Harris. National Institute of Health (R15 program), 2019–2022, $340,000.

Sponsored Program Capacity-Building Activities

1. Communicated (through emails, phone calls and face-to-face meetings) with NIH program officers Dr. David Filpula and Dr. Ravi Veerasamy.
2. Attended the MIDAS (Models of Infectious Disease Agents Study) network meeting and workshop sponsored by NIH in May 2019.

Michael Danquah

Project Title: "Kinetic and computational elucidation of nucleic acid aptameric binding mechanism for enhanced molecular targeting"

Proposal Submissions

1. Atomistic probing of CD79 apta-marking for enhanced pre-B-ALL diagnosis. Submitted to Prevent Cancer Foundation. $100,000.00. PI: Dr. Danquah & co-PI: Dr. Harris.
2. A portable paper-based aptasensor for rapid and simultaneous detection of multiple food and water-borne pathogens. National Science Foundation. $340,084. PI Dr. Danquah; co-PIs Drs Spratt, Levine and Giles
3. Aptameric targeting of CD19 transmembrane receptors for Acute Lymphoblastic Leukemia therapy. Submitted to St. Baldrick Foundation. $92,240.00. PI: Dr. Danquah & co-PI: Dr. Manoo Bhakta (Erlanger).

Contracts/Awards Received

1. Aptameric targeting of CD19 B-lymphocyte transmembrane receptor via molecular dynamics simulations for acute lymphoblastic leukemia therapy.
2. UTC-UTCOM-Erlanger Collaborative Grant: $25,000.00
3. Dr. Michael Danquah (UTC PI) and Dr. Manoo Bhakta (Erlanger PI)

Sponsored Program Capacity Building Activities

1. I have attended a number of on-campus funding and grantsmanship workshop organized by ORSP and SimCenter.

OVERVIEW OF FY2020 PROJECTS

The following awardees and projects, selected for funding in March 2019, are currently supporting CEACSE's strategic goals and future plans for FY2020. All funded projects were subject to double-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. This process ensures high caliber of funded projects and encourages 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.

Core Competition

Title: Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling
Investigators: Sungwoo Yang (Civil & Chemical Engineering)
Swimlane: Energy & the Environment
Amount: **$**99,959

Abstract:
Two-thirds of the world's population in cities is experiencing a water shortage. Current techniques, such as dewing and fog capture, can be used only in locations where the humidity is high. We propose a novel and efficient zeolite-based water harvesting system. A key innovation is the ability to leverage our development of lightweight carbon network as flexible thermal additive and theoretical model to optimize the design of the water-harvesting process via solving the energy/concentration conservation equations. Our novel approach can achieve effective and efficient water harvesting, with a >2.5x higher energy efficiency compared to conventional water generators. The PI is currently the PI on the UTC Faculty Pre-Tenure Enhancement Program. This project has been a successful interdisciplinary collaboration with researchers in UTC Mechanical Engineering, Civil Engineering, and Computational Engineering and Oak Ridge National Labs. The funds requested here would allow the PI to continue previous research by performing detailed experiments to characterize and enhance the vapor diffusion characteristics (inter-/intra-crystalline diffusion) in carbon network and zeolite composites, which dictate water harvesting rates. The PI also performs systematic optimizations of the overall system architecture by leveraging the team's expertise in the development of high-fidelity adsorption computational models.

Title: Alkynyl tetrafluoro-pyridyl ligands: computational studies, synthesis, and characterization
Investigators: Jared Pienkos (Chemistry & Physics)
Swimlane: Health & Biological Systems
Amount: $73,832

Abstract:
Alkynyl compounds can be used to tune the absorption and emission properties of their corresponding transition metal complexes. Herein, we will describe the computational characterization and the synthesis of electron deficient alkynyl tetrafluoro-pyridyl ligands. Iridium, cobalt, and chromium alkynyl tetrafluoro-pyridyl metal ligand interactions will be modeled using a variety of basis sets and functionals supported by the Gaussian/WebMO interface. Concurrent with these computational studies, representative iridium, cobalt, and chromium compounds will be synthesized. Following their synthesis and characterization, modulation of electrochemical and emissive properties will be performed by exploiting secondary binding sites. All of these interactions will be computationally modeled with the Gaussian/WebMO interface using resources

within the SimCenter. Computational tools used in this project will also be implemented for educational outreach activities within the community.

Title: A study on the local and global effects of polymer entanglement in material properties and biological functions
Investigators: Eleni Panagiotou, Jin Wang (Math), Wang-Yong Yang (Chemistry & Physics), Ethan Hereth, & Abdollah Arabshahi (SimCenter)
Swimlane: Health & Biological Systems
Amount: **$**99,941

Abstract:
This proposed research is focused on making the connection between microscopic and macroscopic properties in polymers and biopolymers. First, we propose to use Molecular Dynamics (MD) simulations of coarse-grained models of linear polymer chains in a melt, for various molecular weights, and examine how the entanglement affects the mechanical properties of the material. We will also examine the role of the fluid-structure interactions, and our results will be compared to experimental data. Our results will show how local/global interactions affect material properties, a fundamental question in materials science and in the study of biological systems like the cytoskeleton. Second, we propose to use MD simulations of RNA, which include expanded r(AUUCU) repeats (responsible for spinocerebellar ataxia) to identify special characteristics of their 3D structure. We also study the dimeric compound 2AU-2 that is known to target the pathogenic RNA and model its binding by accounting for fluid-structure interactions. We use topology to study these and to suggest other molecules that would have the same effect. We check our results experimentally. Our results will show how geometry/ topology can be used to create site-specific molecules and could be applied to other extended repeats and lead to site-specific drug delivery methods.

Title: Simulating bio-environmental interactions using –omics approaches
Investigators: Francesca Leasi (Biology, Geology & Environmental Science), Jejal Bathi (Civil & Chemical Engineering), Lani Gao (Math), & Hong Qin (Computer Science & Engineering / Biology, Geology & Environmental Science)
Swimlane: Health & Biological Systems
Amount: $100,000

Abstract:
Biological community assemblages are diverse, maximizing opportunities for species-specific responses to individual components of contamination, and community changes are highly specific to the type and severity of contamination, as well as the interaction of the two. However, there is still a lack of efficient and thoroughly tested statistical models that can be used to identify implicated ecological and trophic features. The goal of this project is to build mathematical models to further our understanding and prediction of the structure, function, and shifting of biological communities in aquatic ecosystems. The proposed approach is driven by recent advances in DNA sequencing technology and represents a potentially transformative application of those advances to environmental simulation and modeling. The study will contribute to fundamental knowledge of ecosystem interactions and how communities respond to disturbance. This project fosters collaboration among researchers in environmental engineering, biology/environmental science, biostatistics, and computational biology and provides interdisciplinary research opportunities for both undergraduate and graduate students. The combined results of this study will be used to develop simulation models using large, biologically realistic data sets with known gene-gene and gene-environment interactions that influence the risk of a complex ecosystem.

Title: Decentralized and Scalable Trust Management Approach via Blockchain for Connected Vehicles in Smart Cities
Investigators: Farah Kandah (Computer Science & Engineering) & Mina Sartipi (Center for Urban Informatics & Progress / Computer Science & Engineering)
Swimlane: Smart Cities & Urban Dynamics
Amount: $100,000

Abstract:
Intelligent transportation system/Connected vehicles are among the key components contributing to the Smart Cities, where vehicles are able to sense their surroundings and communicate with their peers, roadside units, and the infrastructure to share vital transportation information such as road conditions, crashes, and traffic jams. The advancement in this technology creates new cybersecurity requirements, where collaborative entities such as connected vehicles are required to maintain a high level of trust among them to ensure the validity and the credibility of the messages exchanged in the network. Therefore, there is both acritical and urgent need to design, prototype, validate, and demonstrate an integrated system that is better able to build a distributed, tamperproof, and consistent trust-based management system that is able to validate the trust among network entities to add a dimension of assurance, and to ensure that the exchanged data has a quantitative metric of trustworthiness, which will play a vital role in maintaining the safety of the system. 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 vehicle industry.

Title: Corrosion modeling of magnesium-based fixation hardware for mandibular reconstruction surgeries
Investigators: Hamdy Ibrahim & Mohammad Mahtabi (Mechanical Engineering)
Swimlane: Health & Biological Systems
Amount: $94,906

Abstract:
Standard-of-care fixation hardware used for orthopedic skeletal fixation applications are made of stiff metallic alloys that result in several long-term problems such as stress shielding, tissue irritation, and subsequent fixation failure. These poor clinical outcomes often require a second fixation removal surgery. The use of biodegradable fixation hardware made of magnesium that can offer the required stability during the healing period and subsequently degrades is expected to solve these problems and result in a clinical breakthrough. Despite the current interest in biodegradable bone implants, there is still a need to assess the biomechanical performance of these new devices for various bone fixation applications while considering the effect of degradation. In this study, we propose to develop a subroutine and a continuum damage mechanism (CDM) FE model to phenomenologically predict the corrosion rate of our strengthened biocompatible Mg-Zn-Ca-Mn alloy. The developed FE model parameters will be calibrated by conducting a series of in vitro tests on our Mg alloy in conditions simulating the physiological environment. Finally, the developed FE model will be used to compare the biomechanical performance of our Mg alloy with that for an off-the-shelf fixation hardware using a previously-developed 3D model for a mandibular reconstruction surgery.

Title: Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies
Investigators: Azad Hossain, Mark Schorr (Biology, Geology & Environmental Science), & Jejal Bathi (Civil & Chemical Engineering
Swimlane: Energy & the Environment
Amount: $96,488

Abstract:
Satellite observations have been used for water quality studies for many years, but they provide only surface observations and challenges related to cloud coverage and ground truthing, and variable spatial and temporal resolutions remain. Numerical models can provide hydrodynamically computed water quality data on the water surface as well as in the water column, but they have issues with initializations, boundary conditions, calibration, and validation. Although both methods have weaknesses, when used together, they can become a powerful tool to study surface water quality. The proof of concept of this capability was demonstrated in Enid Lake, MS, Lake Pontchartrain, LA, and the Mississippi River using CCHE2D Flow and Water Quality models developed in the National Center for Computational Hydroscience and Engineering at the University of Mississippi. The proposed study aims to further explore this capability at the University of Tennessee at Chattanooga by using the EPA's Better Assessment Science Integrating Point and Non-point Sources (BASINS) model coupled with NASA's Earth observation satellite imagery and near-real-time field measurements to study the spatio-temporal variability of hydrodynamically computed surface water quality parameters in the watersheds of southeast Tennessee.

Title: The Use of Augmented Reality–Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation
Investigators: Jennifer Hogg, Shellie Acocello, Gary Wilkerson (Health & Human Performance), Yu Liang, & Dalei Wu (Computer Science & Engineering)
Swimlane: Health & Biological Systems
Amount: $90,538

Abstract:
Ways in which the neuromuscular system can be leveraged to prevent both initial musculoskeletal and concussive injury and re-injury has been a key area of focus in the literature due to poor injury outcomes. Recent advances in scientific thought suggest that the central nervous system and neurocognition play a greater role in peripheral neuromuscular control than was previously assumed, which presents an opportunity for the development of injury management programs. Because the brain is highly plastic and therefore trainable, research in this area will allow clinicians to take advantage of the brain's modifiable characteristics and devise rehabilitation strategies to improve both lower extremity injury outcomes and post-concussion management. The use of augmented reality–delivered, real-time feedback may serve to improve biomechanical and cognitive outcomes. The current proposal aims to fill that gap by determining the efficacy of using augmented reality to deliver movement feedback and the effect of the delivered feedback on neuromuscular activation, movement kinematics, and cognitive flexibility. Doing so will allow future studies to use the identified parameters to ultimately develop effective injury reduction and management programs.

Title: The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence
Investigators: Bradley Harris (Civil & Chemical Engineering), David Giles (Biology, Geology & Environmental Science), & Ethan Hereth (SimCenter)
Swimlane: Health & Biological Systems
Amount: $92,742

Abstract:
Bacterial pathogens are increasingly developing resistance to conventional antibiotics and represent a mounting threat to public health worldwide. This trend is due in part to the ability of these microorganisms to sense and adapt to their environment through endogenous membrane remodeling strategies. However, the ability of bacteria to adapt their membranes through uptake and assimilation of exogenous fatty acids remains largely unexplored. This project aims to quantify the extent to which exogenous fatty acids contribute to bacterial survival and persistence

and to determine the molecular mechanisms by which fatty acid assimilation impacts membrane behavior. Uncovering this information will vertically advance our understanding of how fatty acids may serve as vital molecules that guide bacterial environmental adaptation and pathogen success. This research could also lead to the development of novel preventatives and therapeutics for antibiotic-resistant infections. Overall, the proposed project will contribute to capacity building and strategic excellence in computational science at UTC and potentially improve public health at large.

Faculty Initiation and Opportunity Award Competition

Title: Models of speciation based on the evolution of electric communication in weakly electric fishes (*Gymnotiformes*)
Investigator: Dr. Fernando Alda-Pons (Biology, Geology, & Environmental Science), Faculty Initiation Award
Swimlane: Health & Biological Systems
Amount: $24,949 (plus $5,000 from startup funds)

Summary:
Freshwater fishes represent a disproportionate amount of the diversity of vertebrates, raising questions on the mechanisms that have originated such a large number of species. In stream fish, vicariance and drift are the main drivers of speciation. This mechanism contrasts to marine fish where adaptation and natural selection prevail, and to other vertebrates (e.g. birds, amphibians), for which species isolation depending on their mating calls have been extensively studied. The main goal of this project is to create a model of incipient speciation based on the evolution of unique electric communication behaviors in Neotropical gymnotiform fish. The approach will combine massive parallel sequencing technologies and bioinformatic tools to simulate evolutionary scenarios that could also be applied to other systems. Ultimately it will advance our understanding on the mechanisms that drive speciation and particularly on the relative roles of neutral and adaptive forces. This study will establish best practices in the field and for computational analyses. It will set the ground for future studies promoting collaborations among evolutionary biologists, ecologists and computer scientists, and will provide opportunities for international relationships involving undergraduate and graduate students.

Title: A simplified subsurface characterization for local-scale groundwater flow models in unconfined sand and gravel aquifers
Investigators: Dr. Stephanie DeVries (Biology, Geology, & Environmental Science), Faculty Initiation Award
Swimlane: Health & Biological Systems
Amount: $24,981 (plus $5,000 from startup funds)

Summary:
The objective of this research is to introduce and test two novel methods for characterization of subsurface properties in unconfined sand and gravel aquifers. These methods will have direct application to the development of local-scale 3D groundwater flow models that can be used to inform water and land-management decisions for municipal well systems. Both methods are based upon data that is readily available as part of a geospatial database of well-construction reports and yield potential to significantly reduce time and labor costs typical of more complex subsurface characterization methods, which makes modeling a more accessible tool for small municipalities to include in source water protection planning. Confidence in these methods as a reliable means of developing small groundwater flow models will be established by performing a statistical comparison of capture zones delineated from models developed using these and previously accepted geostatistical and geologic framework subsurface characterization methods.

Title: Using computational approaches to enhance comparative studies of social evolution
Investigators: Dr. Loren Hayes (Biology, Geology, & Environmental Science), Faculty Opportunity Award
Swimlane: Health & Biological Systems
Amount: $17,242 (plus $500 from the Vice Chancellor for Research and $1,135 from Biology, Geology, & Environmental Science)

Abstract:
Animal social systems (societies) are remarkably diverse. Comparative studies that track the evolution of behavior have revealed important insights into why there is so much variation among species. Despite evidence of intraspecific variation in social systems, most comparative studies have relied on datasets based on the assumption that all species have one form of social organization (e.g., live alone or in groups, not both). Failure to account for intraspecific variation in comparative studies leads to spurious conclusions about social evolution. Building datasets that account for intraspecific variation is time-consuming. Data collection requires manual searches and the extraction of data from thousands of published papers, a process that can take months or years to complete depending on the number of species under investigation. To improve efficiency, we will develop and test programming code for keyword searches of mammalian social systems. We will focus on the artiodactyls, a group of mammals consisting of 226 species. We will compare results collected by automated searches to previously collected data using completely manual searches. To broaden impact, we will also develop a website at which scientists interested in social organization can deposit information. Products will be used to leverage funding from NSF Behavioral Systems.

Title: Modeling of microbial mat decay and implications for the early Earth fossil record
Investigators: Dr. Ashley Manning-Berg (Biology, Geology, & Environmental Science), Faculty Initiation Award
Swimlane: Health & Biological Systems
Amount: $15,000 (no matching)

Abstract:
Microbial mats are organic sedimentary structures that represent Earth's earliest ecosystems. Evidence for ancient microbial life can be found in 3.5 billion-year-old rocks, and in most cases, evidence is based solely on the morphology of the fossil. Many of the best fossils are preserved in microcrystalline silica, which would have required rapid silica precipitation early in the rock forming process before the microorganisms were significantly altered by decomposition. Taphonomic laboratory studies grow monocultures of cyanobacteria that are analogous to the cyanobacteria found in the fossil record and monitor changes to the morphologies of the organisms as they decompose. However, the effects of decomposition on microbial mat preservation are unknown because growing microbial mats in a lab is difficult and time consuming. The proposed research will model microbial mat decay over time and use that model to predict the range of microfossil morphologies that would be observed in the rock record. Biomass accumulation within a mat will be calculated using a previously developed model and used in decomposition models to establish a relationship between biomass and time. The quality of microbial preservation can then be predicted based on the amount of time the mat was exposed to decomposition.

Title: A multi-fidelity computational modeling strategy for large-eddy simulation of turbulent combustion
Investigators: Dr. Reetesh Ranjan (Mechanical Engineering), Faculty Initiation Award
Swimlane: Aerospace & Defense
Amount: $25,000 (plus $5,000 from Mechanical Engineering)

Abstract:
Reacting flows observed in energy conversion and propulsion devices are inherently turbulent and multi-physics in nature. Such flows exhibit interplay of various processes such as reactions, mixing, compressibility, evaporation, and thermal expansion with turbulence, which makes their numerical investigation extremely challenging. Although large eddy simulation (LES) is a promising approach for modeling of such flows, there are still challenges that need to be addressed for improved predictive capabilities. The proposed research focuses on two key challenges faced by LES. The first challenge is related to the validity of the subgrid closures used by LES under different operating conditions, and the second is related to a prohibitive computational cost for design studies. In the proposed work, a multi-fidelity modeling strategy for finite-rate kinetics based LES will be established by employing a modular multi-scale subgrid closure, and nonlinear reduced-order modeling (ROM) technique for efficient design studies. While the emphasis of the physics-based subgrid closure will be on accurately capturing the subgrid turbulence-chemistry interactions, the nonlinear ROM will be evaluated for its ability to efficiently simulate reacting turbulent flows. The proposed multi-fidelity strategy will be evaluated through well-established numerical and experimental test cases corresponding to turbulent premixed combustion.

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 FY2019 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 PhD 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 BS, MS, and PhD Degrees from Caltech. His PhD 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 PhD 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.

Appendix A
Faculty Biosketches

MOHAMMAD AHMADI, Ph.D.
Guerry Professor of Statistics & Management Science

College of Business
The University Of Tennessee at Chattanooga
Chattanooga, Tennessee 37403

EDUCATION

Ph.D.	North Texas State University, Denton, Texas (1976)
Major:	Management Science Minors: Computer Science and Economics Dissertation: *A Study of Economic Development and the Formulation of a Simulation Model of the Economy of Iran.*
M.B.A.	Nicholls State University, Thibodaux, Louisiana (1970) Concentration: Management and Quantitative Methods
B.S.	Mississippi State University, Starkville, Mississippi (1968) Major: Mechanical Engineering

PROFESSIONAL EXPERIENCE

9/2000 to Present	Alexander and Charlotte Guerry Professor, College of Business The University of Tennessee at Chattanooga, Chattanooga, Tennessee 37403
9/82 to 9/2000	Henry Hart Professor, College of Business Administration The University of Tennessee at Chattanooga, Chattanooga, Tennessee 37403
1974 to 1979	Associate Professor, School of Business and Public Administration California State University Bakersfield, California 93309

SELECTED PUBLICATIONS

Published journal articles

"A SWOT Analysis of Big Data," *Journal of Education for Business, Volume 91, Issue 5. 2016.* (Co-authors: Dileepan & Wheatley).

"Predicting Demand for Interlibrary Loan Requests," *The Bottom Line: Managing Library Finances, Volume 26, Issue 3, 2013. (Co-authors: Dileepan & Murgai).*

"Using Control Charts to Monitor Students' Grades When Using A Weighted Average," *International Journal of Multidisciplinary Research, Vol.3 (10), October (2013). Co-author: Deborah Shepherd.*

"A Simulation Model of the Arrival, Flow, and Usage Pattern of Library Resources by the Patrons. Accepted for publication in "*The Bottom Line: Managing Library Finances"*. (Volume 25, Number 4 2012-Co-authors *Dileepan, Murgai)*

"Testing the Transformation Hypothesis of Information and Communications Technologies (ICTs)." *SAM: Advanced Management Journal* (Summer Issue, 2012- *Co-Authors: Laudeman and Helms*)

"The Effect of Custom Song Compositions on Brand Personality: An Empirical Study" *The International Journal of Business, Marketing, and Decision Sciences (Spring 2012. Co-authors: Saulpaugh and Huffman).*

"Quality as a Gap Analysis of College Students' Expectations." *Quality Assurance in Education. Volume .19, Number 4, 2012. (Co-Authors Jackson and Helms)*

"Course 360:-Business statistics, an online course." *Cengage Learning (2012).*

BOOKS

Ahmadi, Mohammad*, Statistics for Business and Economics: A Study Guide and Workbook with Excel Instructions and Examples (ISBN 978-1-4652-6885-3) Kendall Hunt Publishing Company (2016).*

Ahmadi, Mohammad, *Student Workbook to Accompany Statistics for Business and Economics*, West Publishing Company, First Edition (1981), Eleventh Edition (2010).

Ahmadi, Mohammad, *Workbook to Accompany the Essentials of Statistics for Business and Economics,* First Edition (1997) West Publishing Company, Fourth Edition (2006) South-Western College Publishing, An International Thomson Publishing Company (ITP).

PROFESSIONAL ACTIVITIES

Consultant to numerous firms such as Chambliss, Bahner & Stophel; Summers and Wyatt, P.C; Baker, Donelson, Bearman: Caldwell & Berkowitz, P.C.; Erlanger Medical Center; National Seating Company; Chattanooga Paper Board; U.S. Xpress Enterprises, Inc., and many others.

Recent Honors and Recognitions

UT Alumni Association's Outstanding Professor of the Year Award (2017), Scrappy's Professor of the Year Award (2015)

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 91 Reports and Publications):

1. Arabshahi, A., Webster, S.R., Sreenivas, K., “Computational Simulation of the Aerodynamic Environment of Hypersonic Flight Vehicles,” Submitted to the 2018 AIAA Aviation and Aeronautics Forum and Exposition, Atlanta, GA, June 25-29, 2018.
2. 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," the 55th AIAA Aerospace Sciences Meeting, AIAA Science and Technology Forum and Exposition 2017.
3. 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.
4. 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.
5. 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.
6. 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.

7. 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.
8. 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.
9. 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
10. 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.
11. 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 60):

1. Sub-contract from The University of Dayton Research Institute, “Reusable Hypersonic Vehicle Structures,” Co-PI, $893,239.00, October 1, 2017 to September 30, 2020; Funded.
2. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs Computational," Co-PI, $95,220.00, July 2017–June 2018; Funded.
3. Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering, "Laminar-Turbulent Transition Modeling in Navier-Stokes Computations," PI, $92,497.00, July 2017–June 2018; Not Funded.
4. 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.
5. 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.
6. 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, $96,573.00, July 2016–June 2017; Funded.
7. 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.
8. 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.
9. 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.
10. 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.

JEJAL REDDY BATHI
Visiting Assistant Professor
Department of Civil and Chemical Engineering
University of Tennessee at Chattanooga
Chattanooga, TN 37403

A. Professional Preparation:

Osmania University, Hyderabad, India	Chemical Technology	BS	2000
National University of Singapore	Environmental Engineering	M.S.	2005
University of Alabama, AL	Environmental Engineering	M.S.	2007
University of Alabama, AL	Civil Engineering	Ph.D.	2008
University of Alabama, AL	Stormwater Quality	Post-doctoral Fellow	2013 - 2014

Appointments:

2017 – Present	Visiting Assistant Professor University of Tennessee at Chattanooga, TN
20017 – Present	Principal Engineer Syntec Consultants, LLC, TN
2009 – 2016	Principal Civil Engineer Global Systems International, LLC, AL
20014 – 2015	Research Scientist Jackson State University, MS
2013 – 2015	Adjunct Faculty Jackson State University, MS
2006 - 2008	Graduate Research Assistant NSF ALEPSCoR Center for Optical Sensors and Spectroscopies, University of Alabama

Publications and Technical Reports Most Closely Related to the Proposed Project:

1. Bathi, J.R., and H.S. Das**.,** **"**Vulnerability of Coastal Communities from Storm Surge and Flood Disasters," International Journal of Environmental Research and Public Health, Vol. 13, pp 239, 2016.
2. Bathi, J.R., "Black Warrior River hydrodynamics and pollutant transport modeling using a three Dimensional Environmental Fluid Dynamic Code (EFDC)," a technical report submitted to Birmingham Water Works Board (BWWB), 2014. (Findings and technical details of the work are confidential)
3. Pitt, R., K. Goodson, O. Ogburn, V. Eppakayala, Bathi, J.R., Wilson, B., Subramaniam, S., and Clark, S., "Identification and Treatment of Emerging Contaminants in Wet Weather Flows," EPA Contract: EP-C-07-014. Office of Research, EPA, 2013. (Research Report)
4. Bathi, J. R., R.E. Pitt, and S.E. Clark., "Polycyclic aromatic hydrocarbons in urban stream sediments," Advances in Civil Engineering, 2012.
5. Pitt, R. Pitt., S. E. Clark, Y. Cai, M. Renee and Bathi, J.R., "Southeastern United States Observations of Stormwater Pollutant Strengths by Particle Size," Journal of Water Management Modeling, 2017, DOI: 10.14796/JWMM.C418.

5 Other Significant Publications:

1. Bathi, J. R., R. E. Pitt, and S. E. Clark., "Effects of Sediment Characteristics and Location on Polycyclic Aromatic Hydrocarbon (PAH) Associations," International Journal of Environmental Pollution and Solutions, Volume 1.3 (2013), pp 110-130, 2013.
2. Eppakayala, V.J., Bathi, J. R., R. Pitt, S. E. Clark. "Stormwater Treatment at an Industrial Site using a Dry Infiltration Pond with Pre-Treatment". International Low Impact Development Conference 2015, Houston, TX, January 19 – 21, 2015.
3. Bathi, J. R., R. Pitt, S. E. Clark., "Associations of PAHs with Size Fractionated Sediment Particles." World Environmental & Water Resources Congress 2009, American Society of Civil Engineers (ASCE) - EWRI. Kansas City, MO. May 17 – 21, 2009.
4. Gadhamshetty, V., Shrestha, N., Chilkoor, G., Bathi, J.R., "Emerging Environmental Impacts of Unconventional Oil Development in the Bakken Formation in the Williston Basin of Western North Dakota,,,,," In Hydraulic Fracturing: Environmental Issues, Drogos, D. L., Ed., ACS Symposium Series 1216; American Chemical Society, Washington, DC, 2015, Chapter 7.
5. Bathi, J. R., R. Pitt, R. Findlay, S. E. Clark. "Analyses of PAHs in Urban Stormwater Particulates." 11th International Conference on Urban Drainage, 11ICUD. Edinburgh, Scotland, UK, August and September 2008.

Synergistic Activities (up to 5):

1. Reviewer, U.S. Environmental Protection Agency (EPA) Science to Achieve Results (STAR) Fellowship Program, 2015
2. Member, Urban Watershed Management Committee, Environmental and Water Resources Institute of the American Society of Civil Engineers, 2009
3. Member, Publications Committee, Water Environment Federation, 2009
4. Member, Students and Young Professional Committee, Water Environment Federation (WEF), 2007 – 2015
5. Founding Member, Secretary/Treasurer of Black Warrior Environmental Association (BWEA), Student chapter of Alabama Water Environmental Federation and WEF, 2007 – 2008

Jennifer Nagel Boyd – Curriculum Vitae

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, (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. **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.
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. 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.
4. 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.
5. **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.

(ii) 5 other significant

1. Turk JR, Alp N, Dattilo A, **Boyd JN** (2017) Cost-benefit analysis of native warm season grasses for transmission line right-of-way revegetation. *Ecological Engineering* 108: 123–131.
2. Wilder L[*], **Boyd JN** (2016) Ecophysiological responses of *Tsuga canadensis* (Eastern Hemlock) to projected atmospheric CO_2 and warming. *Southeastern Naturalist* 15: 69–713.
3. **Nagel JM**[†], Griffin KL (2004) Can gas-exchange characteristics help explain the invasive success of *Lythrum salicaria*? *Biological Invasions* 6: 101–111.
4. **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.

5. **Nagel JM**[†], Griffin KL (2001) Construction cost and invasive potential: comparing *Lythrum salicaria* (Lythraceae) with co-occuring native species along pond banks. *American Journal of Botany* 88: 2252–2258.

[†] *denotes maiden name;* [*] *denotes undergraduate student author;* [**] *denotes graduate 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 11 graduate students at UTC. This research has produced seven published research articles co-authored by students and numerous professional presentations.
2. Institutional service as the Graduate Program Coordinator of the M.S. in Environmental Science program at the University of Tennessee at Chattanooga from 2015–2017.
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. Service as a reviewer of Fulbright environmental science proposals from 2015–2017 and NSF proposals to the Population and Community Ecology and Bioinformatics programs from 2015–2017.
4. Regional professional service as Chair of the Southern Appalachian Botanical Society Study Conference Support Award Committee in 2018, an elected member-at-large of the Southern Appalachian Botanical Society from 2015–2017, 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 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 applications in 2015, and giving interviews in to WUTC (local NPR station) and WDEF (local television station) about the local hemlock woolly adelgid in 2013.

DR. MICHAEL K. DANQUAH

|PhD, BSc (Hons), CPEng, CEng, CSci, FIChemE|

Professor of Chemical Engineering, Department of Civil and Chemical Engineering. College of Engineering and Computer Science, University of Tennessee, 615 McCallie Ave, Chattanooga, TN 37403, United States. Phone: 832-445-8055 Email: mkdanquah@gmail.com

PROFESSIONAL EXPERIENCE

- Professor, Department of Civil and Chemical Engineering, University of Tennessee, Chattanooga. To commence on August 1, 2018.
- Lead Senior Process Innovation Engineer, Microbial Enrichment Technologies. Agricen Sciences. Dallas - Texas. February 2016 – present
- Professor, Department of Chemical Engineering, Curtin University, Malaysia. Jan 2015 – Feb 2017.
- Associate Dean (Research and Development), Faculty of Engineering and Science, Curtin University, Malaysia. Feb 2013 – Feb 2016.
- Leader, Bio-Process Technologies Research Area, Faculty of Engineering and Science, Curtin University, Malaysia. Nov 2012 – Feb 2016.
- Associate Professor, Chemical Engineering Dept, Curtin University, Malaysia. Nov 2012 - Dec 2014
- Research and Development Consultant and Scientist, Technology Innovation for Biomolecule Purification (Monolithic Purification Technology). Kintan Pty Ltd, Australia. Jan 2008 – Dec 2013
- Senior Lecturer, Department of Chemical Engineering, Monash University, Australia. Jan 2011 - Oct 2011.
- Director & Principal Research Fellow, Bio Engineering Laboratory (Large-scale PC2 facility) and Research Group, Chemical Engineering Dept, Monash University, Australia, Jan 2009 - Oct 2011.
- Lecturer, Department of Chemical Engineering, Monash University, Australia. Jan 2009 - Dec 2010.
- Post-Doctoral Research Fellow, Australian Research Council (ARC) Project on Renewable Energy. Department of Chemical Engineering, Monash University, Australia, April 2008 - Jan 2009.
- Assistant Lecturer, Monash University College, Chemical Engineering, Australia. Nov 2007 – Mar 2008.
- Teaching Assistant (Tutor), Chemical Engineering, Monash University, Australia. July 2005 – May 2008.
- Assistant Lecturer (Teaching Assistant), Chemical Engineering Department, Kwame Nkrumah University of Science and Technology, Ghana. July 2004 – April 2005.

EDUCATION & PROFESSIONAL PREPARATION

- Post-Doctoral Research Fellow, Chemical Engineering, Monash University, Australia, Apr 08 – Jan 09.
- PhD (Chemical Engineering) Monash University, Victoria, Australia. 2008.
- MEngSci (Chemical Engineering) Monash University, Australia. Transferred to PhD in April 2006.
- BSc. Hons (First Class Honours) Chemical Engineering, Kwame Nkrumah University of Science and Technology, Ghana. 2004.
- Professional Certificate in Energy Innovation & Emerging Technologies. Stanford University, US. 2016.
- Graduate Certificate in Higher Education. Monash University, Australia, 2011.
- Fellow (FIChemE), Institution of Chemical Engineers, UK, 2014.
- Chartered Engineer (CEng), Engineering Council, UK, 2013.
- Chartered Scientist (CSci), Science Council, UK, 2013.

SELECTED PROJECT FUNDING

- Large-scale (2000 GPD) process development for biological extraction of humic acids from leonardite. Agricen/Loveland Products, United States. $350,000.00
- One-step process for microalgal biodiesel production using Subcritical Water Extraction (SWE) technology. MoSTI eScience fund (2016): $94,000.00.
- Kinetic modelling of aptameric sensing for real time pathogen detection and bioscreening (2014-2017). MOHE, Fundamental Research Grant Scheme (FRGS 1/2014): ~$37,000.00.
- Speciation and kinetic modelling of microalgae cultivation to enhance biomass production (2014-2015). MOHE Fundamental Research Grant Scheme (FRGS 2/2013): $25,000.00.

- Advancing pathogen detection and screening using aptameric molecules (2014-2016). Curtin Research Flagship Programme. Research Grant: $100,000.00.
- Renewable energy from carbon dioxide: Process engineering to obtain bio-oil from algae. ARC Linkage (Round 2). Industrial Partner: Biofuel Pty Ltd. Victoria, Australia (2008-2011).~ $1,000,000.00.
- Multifunctional biodegradable nanoparticles for enhanced delivery of DNA vaccines. ARC Discovery Project 11 (2011-2013). $ 440,000.00.
- DNA Vaccine delivery. Monash Research Acceleration, Monash University, (2011-2012). $ 90,000.00.
- Immobilised microalgae for desalination and wastewater treatment. Monash NSMRF (2011). $20,000.00.
- High throughput continuous purification of plasmid vaccines. Monash NSMRF (2010). $20,000.00.
- Development of gene-based malaria vaccine. NSMRF (2009). $20,000.00.
- Creating Valuable Health Products from Stem Cells: Bioreactor Development for Stem Cell Cultivation. Engineering Small Grant, Monash University (2009). $18,000.00
- Sustainable Creation of Biofuels from Microalgae via Biochemical and Thermochemical Conversions. Monash Engineering Small Grant, (2010). $20,000.00

PATENTS

- Danquah M. K, Chisholm R, Welsh A, Hinchee M. Biological Process and System for Production of Humic-Based Organic Acids. Provisional Patent in preparation by Faegre Baker Daniels LLP (2018).
- Ongkudon C. M, Danquah M. K. Provisional Patent 2011900918 filed by Watermark IAM, titled "A Liquid Chromatography Column" filed in 2011.
- Danquah M. K, Forde G. M. Provisional Patent 201090011 filed by FB Rice Attorneys, titled Plasmid DNA medium filed in 2010.
- Danquah M. K, Forde G. M. PCT patent (PCT/AU2007/001778) filed by GRIFFITH HACK Patent & Trade Mark Attorneys, titled Materials, Methods, and Systems for Purification and/or Separation, 2007.
- Danquah M. K, Forde G. M. Provisional patent 2006906425 filed by Madderns Patent Attorneys for an invention entitled Development of a Monolithic Adsorbent for High Throughput Biomolecule Purification - Chromatography Method 1, 2006.
- Danquah M. K, Forde G. M. Provisional patent 2006906452 filed by Madderns Patent Attorneys for an invention entitled Single-Stage Chromatographic Process for Biomolecule Purification - Chromatography Method 2, 2006.

SELECTED PUBLICATIONS

Selected from over 200 ISI Journal Publications, Book Chapters & Conference Proceedings. H-Index = 31

1. Tan K. X, Danquah M. K, Sidhu A, Lau S. Y, Ongkudon C. M. Biophysical characterization of layer-by-layer synthesis of aptamer-drug microparticles for enhanced cell targeting. Biotech Progress 34(1) (2018) 249-261.
2. Acquah C, Danquah M. K, Chan Y. W, Moy C. K. S, Ongkudon C. M, Lau S. Y. Chromatographic characterisation of aptamer-modified poly(EDMA-co-GMA) monolithic disk format for protein binding and separation, Separation Science and Technology (2018). DOI: 10.1080/01496395.2018.1443139
3. Agyei D, Acquah C, Tan K. X, Hii H. K, Rajendran S. R. C. K, Udenigwe C. C, Danquah M. K. Prospects in the use of aptamers for characterizing the structure and stability of bioactive proteins and peptides in food. Analytical and Bioanalytical Chemistry 410(2) (2018) 297-306.
4. Tan K. X, Danquah M. K, Sidhu A, Yon L. S, Ongkudon C. M. Aptamer-mediated polymeric vehicles for enhanced cell targeted drug delivery. Current Drug Targets 19(3) (2018) 248-258
5. Tan S. Y, Acquah C, Tan S. Y, Ongkudon C. M, Danquah M. K. Characterisation of charge distribution and stability of aptamer-thrombin binding interaction. Process Biochemistry 60 (2017) 42-51
6. Tan K. X, Danquah M. K, Sidhu A, Ongkudon C. M, Lau S. Y. Towards targeted cancer therapy: Aptamer or oncolytic virus? European Journal of Pharmaceutical Sciences 96 (2017) 8-19
7. Tan S. Y, Acquah C, Sidhu A, Ongkudon C. M, Yon L. S, Danquah M. K. SELEX modifications and bioanalytical techniques for aptamer-target binding characterization. Critical Reviews in Anal Chem 46(6) (2016) 521-537
8. Acquah C, Danquah M. K, Agyei D, Moy C. K, Sidhu A, Ongkudon C. M. Deploying aptameric sensing technology for rapid pandemic monitoring. Critical Reviews in Biotechnology 9/18 (2015) 1-13.
9. Acquah C, Danquah M. K, Yon L. S, Sidhu A, Ongkudon C. M. A review on immobilised aptamers for high throughput biomolecular detection and screening. Analytica Chimica Acta 888 (2015) 10-18.

Vahid Rasouli Disfani

Assistant Professor, University of Tennessee at Chattanooga

Education and Training

- **Ph.D., Electrical Engineering, University of South Florida, FL, 2015**
- **M.S., Electrical Engineering, Sharif University of Technology, Iran, 2008**
- **B.S., Electrical Engineering, Amrirkabir University of Technology, Iran, 2006**

Employment History

Assistant Professor**; 8/2017 - Present**

University of Tennessee at Chattanooga, TN

Postdoctoral Scholar**; 8/2015 – 7/2017**

University of California San Diego, CA

Research Assistant**; 8/2012 – 8/2015**

University of South Florida San Diego, FL

Relevant Publications

- **Disfani, V.R., Fan, L., Miao, Z. and Ma, Y., 2015. Fast Model Predictive Control Algorithms for Fast-Switching Modular Multilevel Converters. Electric Power Systems Research, 129, pp.105-113.**
- **Ma, Y., Miao, Z., Disfani, V.R. and Fan, L., 2014, July. A One-Step Model Predictive Control for Modular Multilevel Converters. In 2014 IEEE PES General Meeting| Conference & Exposition. IEEE.**
- **Yanga, D., Quanb, H., Disfani, V.R., and Liud, L., 2017. Reconciling Solar Forecasts: Temporal Hierarchy. Solar Energy.**
- **Babacan, O., Ratnam, E., Disfani, V.R., and Kleissl, J., 2017. Distributed Energy Storage System Scheduling Considering Tariff Structure, Energy Arbitrage and Solar PV Penetration. Solar Energy.**
- **Pecenak, Z.K., Disfani, V.R., Reno, M.J., and Kleissl, J., 2017. Multiphase Distribution Feeder Reduction. IEEE Transactions on Power Systems.**
- **Habib, A.H., Disfani, V.R., Kleissl, J., and de Callafon, 2017. Optimal Switchable Load Sizing and Scheduling for Standalone Renewable Energy Systems. Solar Energy.**
- **Yanga, D., Quanb, H., Disfani, V.R., and Liud, L., 2017. Reconciling Solar Forecasts: Geographical Hierarchy. Solar Energy, 146, pp.276-286.**
- **Pecenak, Z., Kleissl, J. and Disfani, V.R., Smart Inverter Impacts on California Distribution Feeder with Increasing PV Penetration. In 2017 IEEE Power & Energy Society General Meeting. IEEE.**
- **Khazaei, J., Piyasinghe, L., Disfani, V.R., Miao, Z., Fan, L. and Gurlaskie, G., 2015, July. Real-Time Simulation and Hardware-In-the-Loop Tests of a Battery System. In 2015 IEEE Power & Energy Society General Meeting. IEEE.**

Nancy Fell, PT, PhD, NCS Emeritus

University of Chattanooga Foundation Professor
Department of Physical Therapy
University of Tennessee at Chattanooga.
615 McCallie Ave.
Chattanooga, TN 37403
Phone: 423-425-4747
Email: Nancy-Fell@utc.edu

Professional Preparation

St. Louis University	St. Louis, MO	Physical Therapy	BS, 1987
Washington University	St. Louis, MO	Health Science	MHS, 1992
University of Tennessee	Knoxville, TN	Motor Control and Learning	PhD, 2001

Appointments

2013 – Present	Professor Department of Physical Therapy; Adjunct Faculty Occupational Therapy University of Tennessee at Chattanooga, Chattanooga, TN
2005 – 2013	Associate Professor Department of Physical Therapy University of Tennessee at Chattanooga, Chattanooga, TN
1995 – 2005	Assistant Professor (Tenured 2001) Department of Physical Therapy University of Tennessee at Chattanooga, Chattanooga, TN

Proposal-Related Scholarly Products

[1] True H, Fell N, Harris A, Cho J, Hu ZE, Sartipi M. 02/2018. Functional Measurement Post-Stroke via Mobile Technology. Poster presented at the American Physical Therapy Association's Combined Sections Meeting, New Orleans, LA.

[2] Fell N, Sartipi M, True HH, Allen B, Williams B, Harris A, Cho J, Hu Z, Thompson R. 10/2017. Mobile Technology for Post-Stroke Recurrence Prevention and Recovery (mStroke). 1.5 hour symposia presented at the American College of Rehabilitation Medicine's Annual Conference. Atlanta, GA.

[3] Cho JS, Hu Z, Fell N, Heath GW, Qayyum R, Sartipi M. Hospital Discharge Disposition of Stroke Patients in Tennessee. *Southern Medical Journal*. 2017; doi: 10.14423/SMJ.0000000000000694. [4] Fell N, Clark A, Jackson J, Angwin C, Farrar I, Bishop C, Stanfield H. The Evolution of a Community-wide Interprofessional Fall Prevention Partnership: fall prevention as a vehicle for community and university collaboration and interprofessional education. *J Interprofess Ed Practice.* 2017;8:47-51.

[5] Williams B, Allen B, Hu Z, True H, Cho J, Harris A, Fell N, Sartipi M. Real-Time Fall Risk Assessment Using Functional Reach Test. *International Journal of Telemedicine and Applications*. 2017; doi:10.1155/2017/2042974.

Other Significant Products

[1] Sullivan JE, Larsen D, Pinto-Zipp G, Fell N. 11/2016. The Final P: Pearls from the IV STEP Conference. Presentation at the American Congress of Rehabilitation Medicine, Chicago, IL.

[2] Fell N, Mabey R, Mohr T, Ingram D. The Preprofessional Degree: is it an essential doctor of ph ysical therapy education qualification? *J Phys Ther Ed*. 2015;29(3):13-21.

[3] Barlew L, Secrest J, Guo Z, Fell N, Haban G. The Experience of Being Grounded: A phenomenological study of living with a wheelchair. *Rehabil Nurs*. 2013;38(4):193-201.

[4] Fell N, Lopez NA, Abercrombie S, Grisham CE, Kinzalow LL, Pile EM, Samuels SA, Rogers CW. 02/2012. Interrater and intrarater reliability of the Sitting Balance Assessment Tool (SitBAT) in the Skilled Nursing Facility Setting. Platform presented at the American Physical Therapy Association's Combined Sections Meeting, Chicago, IL.

[5] Fell N, Ellison B, Morris E, Ransom B, SanLuis A, Barron D. 02/2011. Interrater and Intrarater Reliability of a Sitting Balance Assessment Tool (SitBAT) with Patients with Acute Nonprogressive Central Nervous System Disorders. Poster presented at the American Physical Therapy Association's Combined Sections Meeting, New Orleans, LA.

Synergistic Activities

[1] Sartipi M, Hu Z, Fell N, Heath G, Qayyum R. 11/2016. $7,500 Collaborative Research Initiative for Sponsored Programs (CRISP), University of Tennessee at Chattanooga. Post Stroke Management Using Historical Health Data and Big Data Analytics

[2] Fell N, Crowe J, Sartipi M, Yang L. 03/2016. $12,457 Alliance of Women Philanthropists, University of Tennessee. Stroke Rehab Exercise Video Production: Resources supporting post-stroke recovery and professional training

[3] Sartipi M, Cao Y, Fell N, Yang L. 05/2014. $386,186 NIH-R15. mStroke: Mobile Technology for Post-Stroke Recurrence Prevention and Recovery.

[4] Lindgren K, Smith C, Schreeder C, Clark A, Fell N, Radu V, White D, Guo Z. 05/2012. $1,438,680 HRSA; Inter-Professional Collaborative Practice Approach for Geriatric Education Strategies.

[5] Lindgren K, Smith C, Jackson J, Clark A, Fell N, Tillman L, Wilkerson G, Colston M, Panda M, Guo Z. 05/2012. $1,088,064 HRSA. Providing Advanced, Culturally Competent Care through Clinical Training for Inter-Professional Geriatric Care.

Ignatius W. Fomunung

a. Professional Preparation

Institution	Major	Degree	Year
Nanjing Institute of Technology	Civil Engineering	B.S.,	1987
Clark Atlanta University	Physics	M.S.,	1995
Georgia Institute of Technology	Transportation Engineering	M.S..,	1996
Georgia Institute of Technology	Civil and Environmental	Ph.D.,	2000

b. Appointments

2016 – Present	***Professor*** – Department of Civil Engineering, UTC, Chattanooga
2015 – Present	***Visiting Professor*** – Changsha University of Science and Technology, China
2005– 2016	***Associate Professor***—Department of Civil Engineering, UTC, Chattanooga
2000 (Fall) –2005	***Assistant Professor***— Department of Engineering Clark Atlanta University
2000 (Jan - July)	***Post-Doctoral Research Fellow—*** Center for Theoretical Studies of Physical Systems, Clark Atlanta University.
2000 (Jan -May)	***Visiting Assistant Professor—***Department of Physics, Spelman College
1996 - 2000	***Graduate Research & Teaching Assistant—*** School of Civil and Environmental Engineering, Georgia Institute of Technology
1988 - 1993	***Civil and Hydraulic Engineer—***Cameroon Development Corporation and Del Monte Foods.

c. Products

PRODUCTS MOST CLOSELY RELATED

1. *Abubakr Ziedan, Ignatius Fomunung, Joseph Owino, Andrew Ray and Melissa Taylo*r. Assessing the impacts of workforce participation rates in telecommuting programs on VMT and emission reductions in a mid-size city. The 22nd International Conference of the Hong Kong Society for Transportation Studies (HKSTS), Hong Kong December 9 -11, 2017
2. *Murad Al Qurishee, Ignatius Fomunung*. Smart Materials in Smart Structural Systems. Imperial Journal of Interdisciplinary Research (IJIR) vol-3, Issue-7, 2017
3. *Ignatius Fomunung, Joseph Owino, Brent Rollins.* Effects of Wax Emulsion Admixture on Compressive Strength and Surface Characteristics of Roller Compacted Concrete. International Journal of Transportation Technology Transfer in Africa (IJT2A) vol. 1, no. 2, Dec. 2014" edition
4. *Joseph Owino, Ignatius Fomunung, Mohammed Khalafala*. The Recent Development in Roller Compacted Concrete. International Journal of Transportation Technology Transfer in Africa (IJT2A) vol. 1, no. 2, Dec. 2014" edition
5. *Ignatius Fomunung, Joseph Owino, Mbakisya Onyango, Ammar El Assan.* Evaluation of Two Pavement Rehabilitation techniques for Municipal Roads, ASCE Geotechnical Special Publications Nos 236-243, Proceedings of the Geo-Shanghai International Conference, Shanghai, Edited by Wenqi Ding, Lianyang Zhang, Xiaojun Li, and Xiong Zhang, China, 2014.
6. *Trisha Sen, Mbakisya Onyango, Joseph Owino, Ignatius Fomunung, Jim Maxwell, Benjamin Byard*. Pavement Management Analysis of Hamilton County Using HDM-4 and HPMA – International Road Federation (IRF) Examiner, Summer 2014

OTHER SIGNIFICANT PRODUCTS

1. *Mark E.Hairr, Ron D. Sweeny, J. Ronald Bailey and Ignatius Fomunung. "*Developing Hydrogen Hybrid ICE and Inductive Power Transfer Technologies for Buses: Chattanooga, Tennessee, USA Continues to Lead in Advanced Transit Technologies After Twenty Years, Proceedings of the 25th World Battery, Hybrid and Fuel cell Electric Vehicle Symposium, Shenzhen, China Nov 2010

2. *Wade Gasior, Li Yang, Ignatius Fomunung, Mark Hairr, J. Ronald Bailey.* Electric Vehicle Visualization and Simulation, Proceedings of the 25th World Battery, Hybrid and Fuel cell Electric Vehicle Symposium, Shenzhen, China Nov 2010

3. *Adjo Amekudzi, and Ignatius Fomunung,* "Integrating Brownfields Redevelopment with Transportation Planning " Journal of Urban Planning and Development (JUPD) Vol. 130 No. 4 (2004), 204 -212**.**

4. *Shauna Hallmark, Randall Guensler, Ignatius Fomunung,* "Characterizing On-road Variables that affect Passenger Vehicle Modal Operation" Transportation Research D 7 (2002), 81-98

d. Synergistic activities

1. Session Chair – 25th World Electric Vehicle and Battery Symposium, November 3 -10, 2010, Shenzhen, China.
2. Session Chair - International Conference on Health Monitoring of Structure, Material & Environment (HMSME 2007), October 16-18, 2007, Southeast University, Nanjing, China
3. Co-Organizer of the NSF sponsored US-Africa Advanced Studies Institute to promote collaboration between US and African Scientists in Durban, South Africa, November, 2005
4. NASA Research Summit, Orlando, Florida, July 16-19, 2003 Steering Committee Member
5. Established and ran the Summer Transportation Institute (USDOT and FHWA) for upcoming 9th and 12th grade students at Clark Atlanta University in 1999.

e. Collaborators & other affiliations

1. **Collaborators**

Owino, Joseph	Professor	University of Tennessee-Chattanooga
Adjo Amekudzi	Professor	Georgia Institute of Technology
Mbakisya Onyango	Associate Professor	University of Tennessee Chattanooga
Weidong Wu	Assistant Professor	University of Tennessee Chattanooga

2. **Graduate advisor**

Simon Washington	Georgia Institute of Technology
Randall Guensler	Georgia Institute of Technology

3. **Thesis advising**

Harry Smithers, … December 2014 – Advisor.

Ammar El Hassan, The Effects of Visual Stability Index (VSI) on Fresh Segregation of Self Consolidating Concrete (SCC), July 2014 – committee member

Gloria Neal, The Physical and Economic Impacts of Urban Flooding on Critical Infrastructure and Surrounding Communities, May 2014;MS Civ Eng. - Advisor

Nick Andrews, Comparing the Design of I-Shape Members Loaded in Tension, Compression, and Flexure Using the 8th Edition and 13th Edition AISC Steel Construction Manual, May 2014; MS Civ Eng. – committee member

Mark Olivier Labrie, Energy Plus Building Conversion; MS Mech Eng. May 2014 – committee member

Trisha Sen, Pavement Management Analysis of Hamilton County Using HDM4 and HPMA; MS Civ E. May 2013 – committee member

Derek Blackwood, Andy Holsted, Eddie Barton, Will Rogers, Hudson Road and Terminal Road Paving Project, City of Chattanooga Public Works Department, December 2008 -Advisor

Seth Campbell, Philip York, Ryan Steiner, Mark Welsh, John Patterson, 5th Street Resurfacing Project, City of Chattanooga, Department of Public Works, May 2008 -Advisor.

Aashish Niphadkar, Travel Time Study for Chattanooga/Hamilton County/North Georgia TPO; MS in Engineering Management, January 2008 – Co-Advisor

Ken Doyle, Speed and Intersection Camera Study, City of Chattanooga Traffic Engineering Office, May 2007- Advisor

ARASH (ARI) GHASEMI
1302 Peter Pan Road
Lookout Mountain, GA 30750
Cell: (423) 999-6541
Email: Arash-Ghasemi@utc.edu

EDUCATION

August 2016 ***Doctor of Philosophy, Computational Engineering***
The University of Tennessee at Chattanooga, Center of Excellence in Applied Computational Science and Engineering
- Graduated with GPA of 4.0 out of 4.0
- *UTC Outstanding PhD Student Award*

May 2013 ***Master of Science, Computational Engineering***
The University of Tennessee at Chattanooga, Center of Excellence in Applied Computational Science and Engineering
- Graduated with GPA of 4.0 out of 4.0

September 2003 ***Bachelor of Science, Aerospace Engineering***
Sharif University of Technology - Tehran, Iran

WORK EXPERIENCE

August 2017 To current ***Director of Civil Engineering Research and Laboratory***
The University of Tennessee at Chattanooga

August 2016 To August 2017 ***Research Intern***
The University of Tennessee at Chattanooga, Center of Excellence in Applied Computational Science and Engineering
Selected Research:
- ParCurvedMesh - A massively MPI Parallel mesh generator for 2D/3D finite and spectral element methods using industrial CAD models (written in C++ and Fortran 2008)
  - Features:
    - Built-in 3D mesh linear generation
    - Distributed parallel interface to CAD engine OpenCASCADE
    - Curved element suitable for arbitrary-order finite elements
    - Improved load balancing based on a new partitioning algorithm Parallel adaptive visualization

January 2011 To August 2016 ***Graduate Research Assistant***
The University of Tennessee at Chattanooga, Center of Excellence in Applied Computational Science and Engineering
Selected Research:
- Codename “Terrible” - A state-of-art highly non-conforming spectral element code library written in Fortran 2008, C, C++ and Python
- ParLU - Large scale MPI parallel LU decomposition of dense matrices using a distributed block cyclic partitioning (written in C)
- Parnoldi - Massively parallel MPI based implementation of Arnoldi iterations for computing eigen values of distributed sparse matrices

- ParGMRES - Massively parallel MPI based implementation of Generalized Minimal Residuals (GMRES) for solving non-symmetric sparse linear systems (written in C) (https://github.com/arrgasm/paraGMRES)
- ns3D - Three-Dimensional Mixed-Element Unstructured Finite-Volume Solver for Compressible Euler/Navier-Stokes Equations (https://github.com/arrgasm/ns3D)
- UnstEuler2D - Completely Validated Unstructured 2D Compressible Euler Solver - CFD (https://github.com/arrgasm/UnstEuler2D)

2008 To 2011 ***Senior Engineer***

Sadra Aerospace Engineering Company - Tehran, Iran

- Design and implementation of the prototype of subsonic tail-controlled missile
- Design of FPGA-based autopilot system
- Design of data logger system using AVR micro-controllers

SELECTED PUBLICATIONS

- Ghasemi and Lafe K. Taylor, "*Preconditioning the iterative solution of Ax=b using a statistical method*", Procedia Computer Science, Volume 80, 2016, Pages 2266-2270.
- A. Ghasemi, L. K. Taylor and J.C. Newman III, "*hp-Spectral Hull: A Minimum Degrees of Freedom Enforcing Spectral Element Method For Nonlinear Conservation Laws with Application to Compressible Fluid Flow*", **AIAA** Aviation and Forum and Exposition Washington 2016, https://doi.org/10.2514/6.2016-3972
- A. Ghasemi, L.K. Taylor and J.C. Newman III, "*An Embarrassingly Parallel Method for Curved Spectral/Finite Element Mesh Generation of industrial CAD geometries without Linear Elasticity in Two and Three Dimensions*", **ASME** Fluid Engineering Division Summer Meeting 2016, *Also will be submitted to* ***ASME*** *Journal of Computing and Information Science in Engineering*
- A. Ghasemi, K. Sreenivas and L. K. Taylor, "*Unconditionally stable high-order picard iteration algorithm for computational electromagnetics*", **IEEE** Antennas and Propagation Society International Symposium (APSURSI), Chicago 2012
- A. Ghasemi and L. K. Taylor, "*A Progressive Statistical Method for Preconditioning Matrix-Free Solution of High-Order Discretization of Linear Time-Dependent Problems*", http://arxiv.org/abs/1308.5626, 2013
- A. Ghasemi, L. K. Taylor and K. Sreenivas, "*Numerical Stability and Catalan Numbers*", http://arxiv.org/abs/1309.4820 2013
- A. Ghasemi, "*Developing Nonlinear ODE Solvers For Practical Simulation of Air Vehicle Configurations Using Compact Schemes for Integration*", **AIAA** Atmospheric Flight Mechanics Conference, Toronto, Ontario, AIAA-2010-7808
- A. Ghasemi, "*Oscillating Pipe Flow: High-Resolution Simulation of Nonlinear Mechanisms*", American Society of Mechanical Engineers (**ASME**), Fluid Engineering Division Conference, Miami, USA (2006),FEDSM2006-98071, pp1-10, ISBN: 0-7918-4750-0
- A. Ghasemi, "*An Optimized Large-Stencil Approach for Capturing Near-PI Frequencies*", 12th AIAA/CEAS Aeroacoustics Conference, **AIAA**2006-2634, Massachusetts, USA
- A. Ghasemi, "*Strongly Nonlinear Two-Dimensional Standing Waves in an Acoustical Resonator*", Proceedings of the 9th Western Pacific Acoustics Conference (WESPAC IX), Seoul, Korea 2006
- A. Ghasemi, "*Numerical Solution of High-Frequency Oscillations of a Gas Column Using a Modified Lax-Wendroff Scheme*", International Conference on Noise and Vibration Engineering ISMA2006, Leuven, Belgium

BIOGRAPHICAL SKETCH
DAVID GILES

(a) Professional Preparation

Institution and Location	Degree	Year	Field of Study
Maryville College, Maryville, TN	B.A.	2001	Biology
East Tennessee State University Quillen COM, Johnson City, TN	Ph.D.	2008	Biomedical Sciences: Microbiology
Georgia Health Sciences University, Augusta, GA	Postdoctoral PI: M. S. Trent	2008-2009	Biochemistry and Molecular Biology
The University of Texas at Austin, Austin, TX	Postdoctoral PI: M. S. Trent	2009-2012	Molecular Genetics and Microbiology

(b) Appointments

August, 2012-Present Assistant Professor, The University of Tennessee at Chattanooga
July, 2008-July, 2012 Postdoctoral Fellow, Section of Molecular Genetics and Microbiology, The University of Texas at Austin
January, 2008-June, 2008 Postdoctoral Fellow, Dept. of Biochemistry and Molecular Biology, Georgia Health Sciences University

(c) Products

(i) Publications Pertinent to Project

Moravec, A. R., A. W. Siv, C. R. Hobby, E. N. Lindsay, L. V. Norbash, D. J. Shults, S. J. K. Symes and **D. K. Giles**. 2017. Exogenous polyunsaturated fatty acids (PUFAs) impact membrane remodeling and affect virulence phenotypes among pathogenic *Vibrio* species. *Appl Environ Microbiol* 83: e01415-17. doi: 10.1128/AEM.01415-17

Pride, A. C., C. M. 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* 4: e00305-13.

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.

Giles, D.K., J. V. Hankins, Z. Guan, and M.S.Trent. 2011. Remodeling of the *Vibrio cholerae* membrane by incorporation of exogenous fatty acids from host and aquatic environments. *Mol. Micro*. 79: 716-728.

(ii) Other Significant Products

Eder, A.E., S. A. Munir, C. R. Hobby, D. M. Anderson, J. L. Herndon, A. W. Siv, S. J. K. Symes and **D. K. Giles**. 2017. Exogenous polyunsaturated fatty acids (PUFAs) alter phospholipid composition, membrane permeability, biofilm formation and motility in *Acinetobacter baumannii*. *Microbiology*. 163:1626-1636.

Needham, B. D., S. M. 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. Sci. USA*. 110: 1464-1449.

Hankins, J. V., J. A. Madsen, **D. K. Giles**, B. M. Childers, K. E. Klose, J. S. Brodbelt, and M. S. Trent. 2011. Elucidation of a novel *Vibrio cholerae* lipid A secondary hydroxyl-acyltransferase and its role in pathogenesis. *Mol. Micro.* 81: 1313-1329.

Cullen, T. W., **D. K. Giles**, L. N. Wolf, C. Ecobichon, I. G. Boneca, and M. S. Trent. 2011. *Helicobacter pylori* versus the host: Remodeling of the bacterial outer membrane is required for survival in the gastric mucosa. *PLoS Pathog*. 7: e1002454.

United States Patent No. 8,945,587 titled ‘Synthetic Lipid Biology For Combinatorial Engineering Of Endotoxin’.

(d) Synergistic Activities

1. Co-PI on NSF grant (#1520672) that seeks to integrate education, research and training for math majors at UTC. Activities include lectures, laboratories and participation in summer I-MATH camp, an interdisciplinary collection of lectures and exercises for high school students.

2. Co-PI on an internally funded grant involving bioreactor-scale simulation of the biphasic lifestyle of *Vibrio cholerae* to study the impact of exogenous fatty acids

3. Co-PI on an internally funded grant involving the characterization of methicillin-resistant *Staphylococcus aureus* from Erlanger Children's Hospital in Chattanooga, TN.

4. Chair of Student Poster and Presentation Awards Committee for Association of Southeastern Biologists.

5. Development of an Honors course titled '*Deja Flu: Intervention and Control of Emerging and Re-Emerging Epidemic Diseases'*

Biographical Sketch: John R. Graef

(a) Professional Preparation

Loyola University, Chicago, IL, B.S. in Mathematics, 1964
St. Mary's University, San Antonio, TX, M.S. in Mathematics, 1965
Southern Illinois University, Carbondale, IL, Ph.D. in Mathematics, 1970

(b) Appointments

The University of Tennessee at Chattanooga
Professor of Mathematics, 2014 - present
Professor of Mathematics and Head of Department, 1999 - 2014

Mississippi State University
Professor of Mathematics, 1979 - 1999
Interim Head, 1996 - 1998
Associate Professor of Mathematics, 1973 - 1979
Assistant Professor of Mathematics, 1970 - 1973

Southern Illinois University
Graduate Teaching Assistant, 1966 - 1970

San Antonio Independent School District
Mathematics Teacher, 1965 - 1966

(c) Publications

Five publications most closely related to the proposal:

1. *Global dynamics of a SEIR model with varying total population size*, with J. Karsai, M. Y. Li, and L. Wang, Mathematical Biosciences 160 (1999), 191–213.
2. *Periodic solutions of some models with strong allee effects*, with S. Padhi and S. Pati, Nonlinear Analysis: Real World Applications 13 (2012), 569–581.
3. *Periodic solutions of a single species renewable resources under periodic habitat fluctuations with harvesting and Allee effect*, with P. K. Kar, S. Padhi, and S. Pati, Communications on Applied Nonlinear Analysis 20 (2013), 1–16.
4. Periodic Solutions of First–Order Functional Differential Equations in Population Dynamics, with S. Padhi and P. D. N. Srinivasu, Springer, New York, 2014.
5. *Stationary solution of a stochastic nosocomial epidemic model in hospital intensive care units*, with L. Kong and M. Wang, Stochastic Analysis and Applications 32 (2014), 840–850.

Five other significant publications:

1. *Functional differential equations with delay and random effects*, with A. Benaissa and M. Benchohra, Stochastic Analysis and Applications 33 (2015), 1083–1091.
2. *Multiple solutions of systems of fractional boundary value problems*, with L. Kong and Q. Kong, Applicable Analysis 94 (2015), 1288–1304.
3. *Positive solutions for a fractional boundary value problem*, with L. Kong and B. Yang, Applied Mathematics Letters 56 (2016), 49–55.

4. *On Urysohn-Volterra fractional quadratic integral equations*, with M. A. Darwish and K. Sadarangani, Journal of Applied Analysis and Computation 8 (2018), 331–343.
5. *The forward and inverse problems for a fractional boundary value problem*, with Y. Feng, L. Kong, and M. Wang, Applicable Analysis, to appear.

(d) Synergistic Activities

- Proposal reviewer for the National Science Foundation, the National Research Council, and several other US and foreign foundations. Editor-in-Chief of *Communications in Applied Analysis*, member of the Editorial Boards of twenty-seven journals, referee for more than ninety journals. Served as external reviewer for tenure and promotion of faculty at other universities, and as an examiner for seventeen Ph.D. students at other universities.
- Designed and teach a course in *Communicating Mathematics* which is required of all undergraduate majors. The course required the preparation and presentation of a research/expository paper by each student. Some of the resulting papers were presented at student paper sessions at regional MAA meetings.
- Designed and conducted a *Graduate Teaching Assistants Workshop* required of all GTAs who had not yet been an instructor of record at MSU. The GTAs lectured from textbooks used for *College Algebra* and *Statistics for the Behavioral Sciences*. Received a Schillig Special Teaching Project Award grant to purchase a video camcorder to videotape the student lectures and give feedback concerning their teachings skills and techniques.
- Hosted a number of mathematicians (at MSU from China, Czech Republic, Greece, Hungary, Russia, Slovakia, and Yugoslavia; at UTC from Belarus, China, Czech Republic, Hong Kong, Hungary, India, Italy, Portugal Scotland, and Turkey) who visited for the purpose of collaborating on joint research. Negotiated a Letter of Agreement between Attila József University (Szeged, Hungary) and MSU to cooperate in areas of research and education. Also negotiated a Letter of Agreement establishing cooperation between Masaryk University (Brno, Czech Republic), the Institute of Mathematics of the Academy of Sciences of the Czech Republic, and MSU in the areas of research and education.
- Have more than 125 co-authors on publications of which more than 30 were students. Served as major professor for six Ph.D. students, one M.S. and three M.A. students; served as minor professor for more than fifty M.S. and Ph.D. students

BIOGRAPHICAL SKETCH *for* SUMITH GUNASEKERA

Personal:

- Name: Sumith Gunasekera
- Position: Associate Professor of Statistics in the Department of Mathematics at The University of Tennessee at Chattanooga (UTC)

Education:

- University of Nevada at Las Vegas (UNLV), Las Vegas, Nevada, USA
  Ph.D., Statistics, August 2009
- University of Colombo (UC), Colombo 3, District of Colombo, Western Province, Sri Lanka
  B.Sc. (Honors), Physics, October 1995
- Engineering Council Certificate: Engineering Council (EC) (Formerly Council of Engineering Institutions (CEI) Examination, London, England, an autonomous region in the country of The Great Britain under the Sovereign State of The United Kingdom, August 1991

Professional Experience:

- Associate Professor of Statistics/Mathematics: Department of Mathematics, UTC (Tenured Graduate Faculty): 2015 – Present
- Assistant Professor of Statistics/Mathematics: Department of Mathematics, UTC (Tenure-track Graduate Faculty): 2009 – 2015
- Graduate Teaching Assistant: Department of Mathematical Sciences, UNLV: 2001– 2009
- Assistant Lecturer: Department of Physics, UC: 1995 –1997

Achievements

- Received the Award for the Outstanding Research & Creative Achievements – 2017, College of Arts & Sciences (CAS) at The University of Tennessee-Chattanooga.

- Merits: Exceed Expectation in the EDO (Evaluation by Development Objectives) granted by the Provost and Senior Vice Chancellor for Academic Affairs on the recommendations by the Head of the Department of Mathematics and the Dean of the College of Arts & Sciences at The University of Tennessee-Chattanooga for the academic year 2015/2016 in 2017.

- The Doctoral Student with the Highest Overall GPA of 3.91 in the Department of Mathematical Sciences, College of Sciences at the University of Nevada-Las Vegas, Nevada, USA (2009).

Publication (Selected):

Papers published, accepted for publication, and in print

1. **Gunasekera, S.** and Wijekularathna, D. K. (2018). Generalized Confidence Limits for the Performance Index of the Exponentially Distributed Lifetime. *Communications in Statistics – Theory and Methods* Published online 0(0), 1–19. Crossref doi link: https://doi.org/10.1080/03610926.2018.1435810

2. **Gunasekera, S.** (2018). Inference for the Burr XII Reliability under Progressive Censoring with Random Removals. *Mathematics and Computers in Simulation* 144, 182–195. Crossref doi link: https://doi.org/10.1016/j.matcom.2017.07.011

3. **Gunasekera, S.** (2017). Bayesian Inference for a Common Scale Parameter of Several Pareto Populations. *Communications in Statistics–Theory and Methods* **46**(6), 2780-2800. Crossref doi link: http://dx.doi.org/10.1080/03610926.2015.1048890

4. **Gunasekera, S.** (2017). Inferences on Functions of Pareto Parameters with applications to Income Inequality. *Communications in Statistics–Simulation and Computation* **46**(2), 933-947. Crossref doi link: http://dx.doi.org/10.1080/03610918.\\2014.983653

5. **Gunasekera S.** (2016). Bayesian Inference for the Offered Optical Network Unit Load. *Communications in Statistics–Theory and Methods* **45**(10), 2890-2919. Crossref doi link: http://dx.doi.org/10.1080/03610926.2014.892136

6. **Gunasekera, S.** (2016). Generalized Inferences for the Expected Winning Bids. *American Journal of Mathematical and Management Sciences* **35**(4), 309-326.
Crossref doi link: http://dx.doi.org/10.1080/\\01966324.2016.1202162\

7. **Gunasekera, S.** (2015). Generalized Inference of R = Pr(X > Y) for Pareto Distribution. *Statistical Papers* (née *Statistische Hefte*) **56**(2), 333-351.
Crossref doi link: http://dx.doi.org/10.1007/s00362-014-0584-8

8. **Gunasekera, S.** and Ananda M. M. A. (2015). Generalized Variable Method Inference for the Location Parameter of the General Half-Normal Distribution. *Journal of Statistical Computation and Simulation* **85**(10), 2115-2132.
Crossref doi link: http://dx.doi.org/10.1080/00949655.2014.923424

Editorial Boards of Journals:

Associate Editor: *Journal of Mathematics and Statistics (JMS)*
International Journal of Multidisciplinary Research and Development (IJARD)
International Journal of Academic Research and Development (IJARD)
International Journal of Advanced Scientific Research (IJASR)
International Journal of Multidisciplinary Education and Research (IJMER)
International Journal of Advanced Educational Research (IJAER)
International Journal of Environmental Sciences & Natural Resources (IJESNR)
International Journal of Statistics in Medical & Biological Research (IJSMBR)

Reviewer/Referee:

1. *Statistical Papers (SP)*
2. *Mathematics and Computers in Simulation (MCS)*
3. *Journal of Statistical Computation and Simulation (JSCS)*
4. *Journal of Applied Statistics (JAS)*
5. *Model Assisted Statistics and Applications (MASA)*
6. *Journal of Mathematical Analysis and Applications (JMAAST)*
7. *International Journal of Clinical Medicine Research (IJCMR)*
8. *Journal of Mathematics and Statistics (JMS)*
9. *American Journal of Science and Technology (AJST)*

Grants and Proposals:

1. UTC Faculty Grant - April Round, 2016
2. UTC UC Foundation Faculty Research Grant - March Round, 2015; March Round, 2014; March Round, 2012; March Round, 2011; March Round, 2009
3. UTC Faculty Development Grant - April Round, 2014; April Round, 2013; April Round, 2012; April Round, 2011

Dissertation, Thesis, and Project Advisory Committees:

1. Faculty Advisor & Dissertation Advisor: Aruna Saram, PhD Dissertation, Department of Mathematics
Second Doctoral Student in the Computational doctoral program with concentration in Computational & Applied Mathematics – 2019
2. Faculty Advisor & Thesis Advisor: Aaron Fisher, MS Thesis, Department of Mathematics
Most Outstanding Math Graduate Student – 2016
3. Faculty Advisor & Thesis Advisor: Hannah Green, MS Thesis Project, Department of Mathematics
Most Outstanding Math Graduate Student – 2015
4. Faculty Advisor & Project Advisor: Caroline Fraser, MS Thesis Project, Department of Mathematics
Most Outstanding Math Graduate Student – 2014
5. Faculty Advisor & Project Advisor: Shaun Walker, MS Thesis Project, Department of Mathematics
Most Outstanding Math Graduate Student – 2012
6. Faculty Advisor & Project Advisor: Farrah Sadre-Marandi, MS Thesis Project, Department of Mathematics,
First Master's *Student in the Mathematics with concentration in Applied Statistics -2010*
7. Faculty Project Director: Andra Blanariu, BS Departmental Honors Thesis, Department of Mathematics – 2012.

Conference Paper Presentations & Panel Discussions:

1. *Joint Statistical Meetings (JSM):* 2017, 2016, 2015, 2014, 2013, 2012, 2011, 2008
2. *Applied Statistics Symposium (ASS):* 2017, 2016

Biographical Sketch: Dr. Bradley Harris

i. Professional Preparation

Undergraduate	University of TN, Knoxville	Chemical Engineering	B.S. 2008
Graduate	University of TN, Knoxville	Chemical Engineering	Ph.D. 2014

ii. Appointments

2015-Present	University of TN, Chattanooga	Assistant Professor
2010-2014	University of TN, Knoxville	Graduate Research Assistant

iii. Publications

(i) Most Closely Related Products

- Harris, B., Cheng, X., and Frymier, P.D. 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. Characterizing the structure-function relationship that governs electron transport in redox proteins. Abstracts of Papers of the American Chemical Society 2014, 247.
- Harris, B. and Frymier, P.D. Harnessing solar energy through enzyme-mediated protein fusions. Abstracts of Papers of the American Chemical Society 2013, 245.

iv. Synergistic Activities

- Conducting biology-related research in collaboration with the Dept. of Biology, Geology, and Environmental Science and the SimCenter at the University of Tennessee at Chattanooga (UTC).
- Faculty advisor for undergraduate students receiving Provost Student Research Awards to conduct research in collaboration with Dr. Giles from UTC Dept. of Biology.
- Established industry-sponsored senior design projects for the chemical engineering senior design course at UTC in collaboration with local industry partners, including BASF, Chattem Chemicals, Colonial Chemical, TVA, and W.R. Grace and Co.
- Developed bioreactor station for junior-level and senior-level chemical engineering laboratory courses in collaboration with Dr. Giles from UTC Dept. of Biology.
- Received funding from the Tennessee Board of Architectural and Engineering Examiners to purchase equipment for new biology- and nanomaterials synthesis-related stations for the chemical engineering laboratories.

v. Collaborators & Other Affiliations

(i) Collaborators and Co-Editors

- Reed Boeger, University of Tennessee at Chattanooga
- Abigail Doyle, University of Tennessee at Chattanooga
- Dr. Xiaolin Cheng, Ohio State University
- Hunter Eberle, University of Tennessee at Chattanooga

- Jerigray Eduave, University of Tennessee at Chattanooga
- Dr. Paul Frymier, University of Tennessee at Knoxville
- Dr. David Giles, University of Tennessee at Chattanooga
- Dr. Ethan Hereth, University of Tennessee at Chattanooga
- Christopher Purvis, University of Tennessee at Chattanooga
- Cooper Thome, University of Tennessee at Chattanooga
- Andrew Turgeson, University of Tennessee at Chattanooga

(ii) Graduate and Postdoctoral Advisors

- Dr. Paul Frymier, University of Tennessee at Knoxville

(iii) Thesis Advisor and Postgraduate-Scholar Sponsor

- Andrew Turgeson, University of Tennessee at Chattanooga

A.K.M. Azad Hossain, Ph.D.
Assistant Professor
Department of Biology, Geology and Environmental Science
The University of Tennessee at Chattanooga
Phone: (423) 425-4404, Email: azad-hossain@utc.edu

(a) Professional Preparation

University of Dhaka	Geology	Bachelor of Science	1995
University of Dhaka	Geology	Masters of Science	1998
University of Mississippi	Geological Engineering	Masters of Science	2004
University of Mississippi	Geological Engineering	Ph.D.	2008
University of Mississippi (NCCHE)	Postdoctoral Research on the application of GIS/Remote Sensing in Computational Hydroscience		2008-2011

(b) Appointments

Assistant Professor — August 2016- Present
Department of Biology, Geology and Environmental Science
The University of Tennessee, Chattanooga

Visiting Assistant Professor — July 2015 – July 2016
Department of Geology and Geological Engineering
The University of Mississippi

Research Scientist — Sept. 2011–June 2015
National Center for Computational Hydroscience and Engineering
The University of Mississippi

Adjunct Assistant Professor — Dec. 2010 – June 2015
Department of Geology and Geological Engineering
The University of Mississippi

Post Doctoral Research Associate — Aug. 2008 – Sept. 2011
National Center for Computational Hydroscience and Engineering
The University of Mississippi

Geographic Information Systems Technician — Mar. 2007 – Aug. 2008
The University of Mississippi Geoinformatics Center
The University of Mississippi

Research Assistant/Instructor/Teaching assistant — Jan. 2002 – Feb. 2007
The University of Mississippi Geoinformatics Center
The University of Mississippi

Remote Sensing and GIS Analyst — May 1999 – Dec. 2001
Center for Environmental and Geographic Information Services
Dhaka, Bangladesh.

GIS Consultant — Nov. 1998 – Apr. 1999
Center for Environmental and Geographic Information Services
Dhaka, Bangladesh.

(c) Publications (10 out of 15)

(i) Five publications most closely related to proposed project:

- Hossain, A. and Greg Easson, 2015, Potential Impacts of the Growth of a Mega City in Southeast Asia, A Case Study on the City of Dhaka, Bangladesh, in "Handbook of Climate Change Mitigation and Adaptation ", Wei-Yin Chen, John M. Seiner, Toshio Suzuki and Maximilian Lackner MBA. (editors), Springer International Publishing, pp 1-24, Online ISBN 978-1-4614-6431-0.
- Hossain, A., Jia, Y. and Chao, X., 2014, Advances in Application of Remote Sensing Techniques to Enhance the Capability of Hydrodynamic Modeling in Estuary, in '*Remote Sensing and Modeling:Advances in Coastal and Marine Resources*', Charles W. Finkl, and Christopher Makowski (editors), Coastal Research Library (CRL) series, vol. 9, pp. 295-313. Springer International Publishing, ISBN: 978-3-319-06325-6.

- Chao, X., Jia, Y. and Hossain, A., 2016, Numerical Modeling of Sediment Transport and Its Effect on Algal Biomass Distribution in Lake Pontchartrain Due to Flood Release from Bonnet Carré Spillway, Journal of Geoscience and Environment Protection 4(9),pp 64-79.
- Chao, X., Hossain, A., and Jia, Y., 2013, 3D Numerical Modeling of Flow and Pollutant Transport in a Flooding Area of 2008 US Midwest Flood, *American Journal of Climate Change,* 2(2), 116-127.
- Chao, X., Jia, Y., Wang, S.S.Y. and Hossain, A., 2012, Numerical modeling of surface flow and transport phenomena with applications to Lake Pontchartrain, Lake and Reservoir Management, 28(1), 31-45.

ii) Five other significant publications:

- Hossain, A., Easson, G., 2016, Soil Moisture Estimation in South-Eastern New Mexico Using High Resolution Synthetic Aperture Radar (SAR) Data. *Geosciences*, 6(1), 1-20.
- Hossain, A., and Easson, G., 2011, Predicting Shallow Surficial Failures in the Mississippi River Levee System Using Airborne Hyperspectral Imagery, *Geomatics, Natural Hazards and Risk,* 3(1), 55-78.
- Kalyanapu, A., Hossain, A., J. Kim, W. Yigzaw, F. Hossain and C. K. Shum, 2013, Investigating the downstream flood hazards on American River due to changes in Probable Maximum Flood due to effects of Artificial Reservoir Size and Land Use/Land Cover Patterns, *Earth Interactions* (AGU-AMS-AAG),Special Issue, 17(24), pp. 1-24.
- Hossain, A., 2013, Flood Inundation and Crop Damage Mapping: A Method for Modeling the Impact on Rural Income and Migration in Humid Deltas, in '*Climate Vulnerability: Understanding and Addressing Threats to Essential Resources'* Faisal Hossain (volume editor), Roger Pielke Sr. (series editor)*, Vol. 5. pp. 357-374,* Elsevier Inc., Academic Press, ISBN: 9780123847034.
- Hossain, A., Easson G., and Hasan, K., 2006, Detection of Levee Slides using Commercially Available Remotely Sensed Data, Environmental and Engineering Geoscience, 12(3), 235-246. 10.2113/gseegeosci.12.3.235 (Journal cover).

(e) Synergistic Activities

- Taught both undergraduate and graduate courses on GIS, Remote Sensing, and Spatial Analysis. Also taught undergraduate courses on Physical Geology, Historical Geology, and Environmental Geology.
- Served as Co-PI for a Mississippi Water Resources Research Institute (MWRRI) sponsored research project, 'Study Transport Processes of Sediment and Mercury and their Interactions in Large Lakes in Mississippi" conducted at the National Center for Computational Hydroscience and Engineering (NCCHE), The University of Mississippi (3/1/2012-2/28/2013).
- Actively involved advising and mentoring both undergraduate and graduate students. Advised about 30 Freshmen in geological engineering and mentored more than 50 upper level undergraduate students at the Department of Geology and Geological Engineering at the University of Mississippi (UM) to do their class projects in GIS, Remote Sensing, and Spatial Analysis Courses. At UM also advised 3 graduate students. During last one year of working at UTC, mentored 17 undergraduate students to do their class projects in the GIS for Geologists course, 4 undergraduate students to do their Geology Senior Seminar research projects, and one research based independent study undergraduate student. Currently, advising about 15 Geology major undergraduate students and serving as a major advisor of an Environmental Science Master's student.
- Served in departmental hiring committee and promotion tasks committee. Reviewed different journal articles. Reviewed external grants for USGS/NIWR. Helped organizing conference and workshops for NCCHE and School of Engineering at UM.

Biographical Sketch: Farah Kandah

Professional Preparation

The Hashemite University	Computer Science	B.S.	2002
The University of Jordan	Computer Science	M. Sc.	2005
North Dakota State University	Computer Science	PhD	2012

Appointments

2012 - present	Assistant Professor, Computer Science and Engineering, University of Tennessee - Chattanooga
2011 - 2012	Teaching Assistant, Department of Computer Science, North Dakota State University
2009 - 2011	Research Assistant, Department of Computer Science, North Dakota State University
2005 - 2007	Lecturer and Course Coordinator, Computer Science Department, The Hashemite University
2003 - 2005	Research Assistant, Computer Science Department, The University of Jordan

Publications

Five Publications Most Closely Related to the Proposed Project

1. S. Schmitt F. Kandah and M. Akour. Towards smart and dynamic load balancing using software-defined network virtual slicing. In *IEEE Consumer Communications and Networking Conference (CCNC)*, 2018
2. S. Schmitt and F. Kandah. Mitigating denial of service attacks using traffic pattern recognition over software-defined network. In *IEEE Consumer Communications and Networking Conference (CCNC)*, 2018
3. S. Schmitt J. Coleman, F. Kandah and M. Akour. Community trust distribution in vehicle ad-hoc networks. In *New Trends in Information Technology (NTIT-2017)*, pages 1–6, april 2017
4. F. Kandah and J. Whitehead. Trust-based survivability provisioning in wireless mesh networks. *IJIPM: International Journal of Information Processing and Management*, 7:36–47, 2016
5. F. I. Kandah, O. Nichols, and Li Yang. Efficient key management for big data gathering in dynamic sensor networks. In *2017 International Conference on Computing, Networking and Communications (ICNC)*, pages 667–671, Jan 2017

Other Significant Publications

1. F. Kandah and J. Whitehead. Energy-aware multipath provisioning in wireless mesh networks. In *2015 12th Annual IEEE Consumer Communications and Networking Conference (CCNC)*, pages 473–478, Jan 2015
2. F. Kandah, Y. Singh, W. Zhang, and Yulu Ma. Mitigating misleading routing attack using path signature in mobile ad-hoc networks. In *2013 IEEE Global Communications Conference (GLOBECOM)*, pages 617–622, Dec 2013
3. Farah Kandah, Yashaswi Singh, and Weiyi Zhang. Mitigating eavesdropping attack using secure key management scheme in wireless mesh networks. *Journal of Communications*, 7(8), 2012
4. Farah Kandah, Yashaswi Singh, Weiyi Zhang, and Chonggang Wang. Mitigating colluding injected attack using monitoring verification in mobile ad-hoc networks. *Security and Communication Networks*, 6(4):539–547, 2013
5. F. Kandah and A. Powell. Ultimate control and security over data localization in the cloud. In *Computing, Networking and Communications (ICNC), 2015 International Conference on*, pages 123–127, Feb 2015

Synergistic Activities

1. **Membership:** IEEE, IEEE Computer Society and IEEE Communication Society (ComSoc).
2. **Founding Director:** Network Communication Lab (Aug 2012 - Present).
3. **Professional services:** Keynote Speaker (Mid SouthEast ACM Conference, 2016), Session Chair (ICNC 2017, CCNC 2015, ICNC 2015), Chair (International Conference on Communications and Networking in China), Guest-Editor (IEEE Multimedia Communications Technical Committee, Nov 2013), TPC Member (IEEE ICC 2015-2018, IEEE SoutheastCon 2017, IEEE / ACM ICCVE 2012-2016, IEEE CIC/ICCC 2016, INTGAST 2015, ICCME 2015, WCNC 2013-2015, and IEEE Globecom 2011-2013), Journal Reviewer (IEEE Sensor Journal, WILEY's Security and Communication Networks (SCN) Journal, International Journal of Information Processing and Management (IJIPM), Journal of Computer Systems, Networks and Communications (JCSNC), International Journal of Information Security and Privacy (IJISP)).
4. **Awards:** Outstanding Tenured/Tenure-Track Faculty Teaching Computer Science and Engineering Award (2017), Faculty/Teacher of the Year Award, Computer Science and Engineering (2017), Outstanding Researcher, Computer Science and Engineering (2015 2016), Named UC Foundation Assistant Professor, 2014.

HOPE KLUG—CURRICULUM VITAE

PROFESSIONAL PREPARATION

University of Florida	Zoology and Psychology	B.S. 2001
University of Florida	Zoology	Ph.D. 2007
University of Helsinki	Post-doc, Biological & Environmental Sciences	2008-2010
Yale University	Post-doc, Ecology & Evolutionary Biology	2010-2011

APPOINTMENTS

University of Tennessee at Chattanooga	Associate Professor	2016 - present
University of Tennessee at 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 (*UNDERGRADUATE STUDENT)

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.

SYNERGISTIC ACTIVITIES

1- Pre-collegiate Training & Outreach

Aquatic Science Days:

During the summers of 2016 and 2017 I developed and lead a series of aquatic science activities for students from local under resourced, minority-serving high schools. These activities were implemented with ~80 students.

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

For three years (2015, 2016, and 2017), I co-led 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, & Chattanooga Nature Center.

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

During 2012, 2013, 2014, 2015, 2016, and 2017 I lead hands-on, inquiry-based science activities for 150+ 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 15 hours/week for 9 months working with teachers & students in an under-resourced middle school, participated in curriculum development and mentored students, and developed a module that was distributed to local teachers and disseminated online.

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

Undergraduate research:

I have integrated undergraduates in all aspects of my research. I have supervised 65 undergraduates at the Universities of Tennessee at Chattanooga, Florida, and Helsinki and at Yale University. Several students have completed honors theses, five are coauthors on peer-reviewed manuscripts.

3- Professional Service

Editorial board memberships:

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

Reviewer for:

Evolution, Ethology, Proceedings of the Royal Society B, Biology Letters, Oecologia, Behavioral Ecology & Sociobiology, Heredity, Animal Behaviour, Journal of Evolutionary Biology, Journal of Ethology, Oikos, Canadian Journal of Zoology, Journal of Fish Biology , American Naturalist, Journal of Theoretical Biology, Annales Zoologici Fennici, Naturwissenschaften, Trends in Ecology & Evolution, Evolutionary Ecology, Molecular Ecology, Nature Communications, Behavioral Ecology, Ecology Letters, BMC Evolutionary Biology, Ecology & Evolution, Behavioral Processes, Biological Reviews, NSF, Graduate Women in Science, National Geographic Society

Academic Advisor for:

Sigma Beta Rho Multi-cultural fraternity, 2012-present
Women in the Natural Sciences, 2015-present

4- 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 12 countries (US, Finland, Canada, Brazil, France, Italy, UK, Australia, Sweden, Norway, China, Portugal).

5- Public interest

My research has been the focus of more than 21 popular news features since 2007.

Biographical Sketch: Lingju Kong

(a) Professional Preparation

Shandong Normal University, Jinan, China, B.S. in Mathematics Education, 1996
Ocean University of China, Qingdao, China, M.S. in Mathematics, 1999
Northern Illinois University, DeKalb, IL, Ph.D. in Mathematics, 2005

(b) Appointments

The University of Tennessee at Chattanooga, Chattanooga, TN
UC Foundation Professor, August 2014–Present
UC Foundation Associate Professor, August 2010–July 2014
UC Foundation Assistant Professor, August 2009–July 2010
Assistant Professor, August 2005–July 2009

Northern Illinois University, DeKalb, IL 60115
Graduate Teaching Assistant, January 2001–May 2005

Caterpillar Inc., Joliet, IL
Intern, May 2003–August 2003

Ocean University of China, Qingdao, China
Instructor, September 1999–December 2000

(c) Publications

More than 140 papers have appeared in print or are accepted for publication in refereed journals, and several more have been submitted for publication. Co-authored 2 research monographs. Authored or co-authored more than 60 presentations at regional, national, and international meetings on mathematics.

Five publications most closely related to the proposal:

1. J. R. Graef, L. Kong, and B. Yang, Positive solutions for a fractional boundary value problem, *Appl. Math. Lett.* **56** (2016), 49–55.

2. J. R. Graef, L. Kong, and Q. Kong, Multiple solutions of systems of fractional boundary value problems, *Appl. Anal.* **94** (2015), 1288–1304.

3. J. R. Graef, L. Kong, and M. Wang, Stationary solution of a stochastic nosocomial epidemic model in hospital intensive care units, *Stoch. Anal. Appl.* **32** (2014), 840–850.

4. J. R. Graef, L. Kong, and M. Wang, A Chebyshev spectral method for solving Riemann-Liouville fractional boundary value problems, *Appl. Math. Comput.* **241** (2014), 140–150.

5. L. Kong, Existence of solutions to boundary value problems arising from the fractional advection dispersion equation, *Electron. J. Differential Equations*, Vol. **2013** (2013), No. 106, pp. 1–15.

Five other significant publications:

1. L. Kong, Weak solutions for nonlinear Neumann boundary value problems with $p(x)$-Laplacian operators, *Taiwanese J. Math.*, **21** (2017), 1355-1379.

2. L. Kong, Positive radial solutions for quasilinear biharmonic equations, *Comput. Math. Appl.* **72** (2016), 2878–2886.

3. L. Kong, Multiple solutions for fourth order elliptic problems with $p(x)$-biharmonic operators, *Opuscula Math.* **36** (2016), 252–264.

4. L. Kong, Eigenvalues for a fourth order elliptic problem, *Proc. Amer. Math. Soc.* **143** (2015), 249–258.

5. L. Kong, On a fourth order elliptic problem with a $p(x)$-biharmonic operator, *Appl. Math. Lett.* **27** (2014), 21–25.

(d) Synergistic Activities

1. Serving in the Editorial Board of *Differential Equations & Applications*. Being guest co-editor (with M. Wang) for special issues published in the journals of *Dynamic Systems and Applications* and *Communications on Applied Analysis*. Reviewed book proposals for several publishers such as Elsevier, Springer, and World Scientific Publishing Corporation. Refereed research papers for more than 50 journals.

2. Co-organizer (with J. R. Graef and M. Wang) of the *Workshop on Boundary Value Problems and Applications* in the 6th International Conference on Dynamic Systems and Applications & the 5th International Conference on Neural, Pararrel & Scientific Computations, Atalanta, GA, May 27–30, 2015

3. Co-organizer (with J. R. Graef and B. Yang) of the special session *Applications of Functional Analytic Techniques to Nonlinear Boundary Value Problems* in the American Mathematical Society 2012 Fall Southeastern Section Meeting, Tulane University, New Orleans, LA, October 13–14, 2012

4. Co-organizer (with J. R. Graef and B. Yang) of the special session *Topological and Variational Methods for Boundary Value Problems* in the 9th AIMS International Conference on Dynamical Systems, Differential Equations and Applications, Orlando, FL, July 1–5, 2012

5. Co-organizer (with J. R. Graef and B. Yang) the special session *Applications of Differential, Difference, and Dynamic Equations* in the 4th International Conference on Neural, Pararrel & Scientific Computations, Atalanta, GA, August 11–14, 2010

Biographical Sketch
Francesca Leasi, Ph.D.

PROFESSIONAL PREPARATION

University of Modena and Reggio Emilia, Italy	Evolutionary Biology	M.S., 2002
University of Modena and Reggio Emilia, Italy	Biology and Ecology	Ph.D., 2007

University of New Hampshire, NH	Research Associate 2017/18
Smithsonian Institution. D.C.	Research Fellow 2013/17
Academy of Natural Sciences, PA	Research Fellow 2012
Imperial College London, UK	Research Associate 2011
University of Milan, Italy	Postdoc 2007/10

APPOINTMENTS

University of Tennessee at Chattanooga	Assistant Professor	2018-Present

FIVE PUBLICATIONS RELATED TO THE PROPOSED PROJECT

LEASI F, Sevigny J, Laflamme EM, Artois T, Curini-Galletti M, de Jesus Navarrete A, Di Domenico M, Goetz F, Hall JA, Hochberg R, Jörger KM, Jondelius U, Todaro MA, Wirshing HH, Norenburg JL, Thomas WK (In Press) Biodiversity estimates and ecological interpretations of meiofaunal communities are biased by the taxonomic approach. *Nature Communications Biology*.

LEASI F, Andrade S, Norenburg JL (2016) At least some meiofaunal species are not everywhere. Indication of geographic, ecological and geological barriers affecting the dispersion of species of *Ototyphlonemertes* (Nemertea, Hoplonemertea). *Molecular Ecology* 25:1381-1397. DOI:10.1111/mec.13568.

LEASI F, Gaynus C, Mahardini A, Moore NT, Norenburg JL, Barber HP (2016) Spatial and ecological distribution of neglected microinvertebrate communities across endangered ecosystems: Meiofauna in Bali (Indonesia). *Marine Ecology* 37: 970-987. DOI:10.1111/maec.12305.

LEASI F, Norenburg JL (2014) The necessity of DNA taxonomy to reveal cryptic diversity and spatial distribution of meiofauna, with a focus on Nemertea. *PLoS ONE* 9(8): e104385. DOI:10.1371/journal.pone.0104385.

Curini-Galletti M, Artois T, Delogu V, De Smet WH , Fontaneto D, Jondelius U, **LEASI F**, Martínez A, Meyer-Wachsmuth I, Nilsson KS, Tongiorgi P, Worsaae K, Todaro MA (2012) Patterns of diversity in soft-bodied meiofauna: dispersal ability and body size matter. *PLoS ONE* 7: e33801. DOI:10.1371/journal.pone.0033801.

FIVE OTHER SIGNIFICANT PUBLICATIONS

Martínez-Arce A, De Jesús-Navarrete A, González-Medina E, **LEASI F** (In Press) COI gene and algorithmic analyses for species delimitation in marine nematodes. *Thalassas: An International Journal of Marine Sciences.*

LEASI F & De Smet W (Accepted) Rotifer distribution at different salinities in the United States with the description of two new species. *Hydrobiologia.*

Mills S, Alcántara-Rodríguez JA, Ciros-Pérez J, Gómez A, Hagiwara A, Galindo KH, Jersabek CD, Malekzadeh-Viayeh R, **LEASI F**, Lee JS, Mark Welch DB, Papakostas S, Riss S, Segers H, Serra M, Shiel R, Smolak R, Snell TW, Stelzer CP, Tang CQ, Wallace RL, Fontaneto D, Walsh EJ (2017) Fifteen species in one: deciphering the *Brachionus plicatilis* species complex (Rotifera, Monogononta) through DNA taxonomy. *Hydrobiologia* 796: 39-58. DOI:10.1007/s10750-016-2725-7.

LEASI F, Tang CQ, De Smet WH, Fontaneto D (2013) Cryptic diversity with wide salinity tolerance in the putative euryhaline *Testudinella clypeata* (Rotifera, Monogononta). *Zoological Journal of the Linnean Society* 168:17-28. DOI:10.1111/zoj.12020.

Tang CQ, **LEASI F**, Obertegger U, Kieneke A, Barraclough TG, Fontaneto D (2012) The widely used small subunit 18S rDNA molecule greatly underestimates true diversity in biodiversity surveys of the meiofauna. *Proceedings of the National Academy of Sciences of the United States of America* 109: 16208-16212. DOI:10.1073/pnas.1209160109.

SYNERGISTIC ACTIVITIES

2018. Session Chair at the symposium "*Measuring Biodiversity and Extinction – Present and Past".* SICB conference, San Francisco, Jan 3-7.

2018. Co-Organizer of the II Benthic Invertebrate Taxonomy, Metagenomics, and Bioinformatics Workshop (BITMaB). Harte Institute Texas A&M Corpus Christi.

2017. Co-Organizer of the I Benthic Invertebrate Taxonomy, Metagenomics, and Bioinformatics Workshop (BITMaB). Harte Institute Texas A&M Corpus Christi.

2016. Organizer of the Meiofauna Workshop. Achotines Bay (Panama).

2013. Co-Organizer of the Marine Biodiversity Inventory Methods Field Course. Bali (Indonesia).

2010. Co-Organizer of the Meiofauna Workshop. Roscoff (France).

REFEREE FOR BioInvasion Records / Bullettin of Marine Science / Cahiers de Biologie Marine / Diversity / Hydrobiologia / Invertebrate Biology / Invertebrate Zoology / Journal of Biogeography / Journal of Experimental Marine Biology and Ecology / Journal of Limnology / Marine Biodiversity / Marine Biology / Marine Environmental Research / Meiofauna Marina / PloS ONE / Revista de Biologia Tropical / Systematic Biology / The Proceedings of the Biological Society of Washington / Zookeys / Zoologica Scripta / Zoological Journal of the Linnean Society / Zoological Science / Zoologischer Anzeiger / Zootaxa

REVIEWER PANEL

2018. Master Thesis Dissertation Committee for the Environmental Engineering Department. University of New Hampshire.

2017. Travel Award Committee. Benthic Invertebrate Taxonomy, Metagenomics, and Bioinformatics Workshop II.

2017. PostDoc Fellowship Committee. Smithsonian Institution, Department of Invertebrate Zoology.

2016. Travel Award Committee. Benthic Invertebrate Taxonomy, Metagenomics, and Bioinformatics Workshop I.

2013. Grant Committee. Encyclopedia of Life.

Biographical Sketch: Andrew Ledoan

(a) Professional Preparation

San José State University, San José, CA, B.S. in Electrical Engineering, 1993
San José State University, San José, CA, M.S. in Mathematics, 2001
University of Illinois at Urbana–Champaign, Urbana, IL, M.S. in Mathematics, 2006
University of Illinois at Urbana–Champaign, Urbana, IL, Ph.D. in Mathematics, 2007

(b) Appointments

The University of Tennessee at Chattanooga, Chattanooga, TN
Associate Head of Mathematics, 2016–Present
Associate Professor of Mathematics, 2015–Present
Assistant Professor of Mathematics, 2012–2015
Visiting Assistant Professor, 2011–2012

Boston College, Newton, MA
Visiting Assistant Professor, 2010–2011

University of Rochester, Rochester, NY
Postdoctoral Faculty/Visiting Assistant Professor, 2007–2010

University of Illinois at Urbana–Champaign, Urbana, IL
Graduate Teaching Assistant, 2002–2007

San José State University, San José, CA
Lecturer, 2000–2001
Teaching Associate, 1999–2000

Trimble Navigation Limited, Sunnyvale, CA
Senior Software Engineer/Member of Technical Staff, 1994–2000

Orion Instruments Incorporated, Menlo Park, CA
Applications Engineer, 1993–1994

General Magic Incorporated, Mountain View, CA
Assistant Engineer, 1992–1993

(c) Publications

Five publications most closely related to the proposal:

1. K. Ferrier, M. Jackson, A. Ledoan, D. Patel, and H. Tran, The expected number of complex zeros of complex random polynomials, *Illinois J. of Math.* **60** (2017), no. 4, 1–14.

2. A. Ledoan, Explicit formulas for the distribution of complex zeros of a family of random sums, *J. Math. Anal. Appl.* **444** (2016), 1304–1320.

3. D.A. Goldston and A.H. Ledoan, Limit points of the sequence of normalized differences between consecutive primes, *Analytic number theory* (edited by C. Pomerance, M.Th. Rassias), 115–125, Springer International Publishing, Switzerland, 2015.

4. D.A. Goldston and A.H. Ledoan, The jumping champion conjecture, *Mathematika* **61** (2015), Issue 3, 719–740.

5. A. Ledoan, M. Merkli, and S.L. Starr, A universality property of Gaussian analytic functions, *J. Theoret. Probab.*, Vol. 25, no. 2 (2012), 496–504.

Five other significant publications:

1. R. Arindam, A. Ledoan, and A. Zaharescu, Zeros of partial sums of the Dedekind zeta function of a cyclotomic field, *J. Number Theory* 136 (2014), 118–133.

2. D.A. Goldston and A.H. Ledoan, On the differences between consecutive prime numbers, I, *Combinatorial number theory: Proceedings of the "Integers Conference 2011," Carrollton, Georgia, October 26–29, 2011*, 37–44, De Gruyter Proc. Math., De Gruyter, Berlin, 2013.

3. A. Ledoan and A. Zaharescu, The pair correlation of homotetic images of zeros of the Riemann zeta-function, *J. Math. Anal. Appl.* 395 (2012), 25–283.

4. A. Ledoan and A. Zaharescu, Explicit formulas for the pair correlation of vertical shifts of the zeros of Riemann's zeta-function, *Comment. Math. Univ. St. Pauli*, Vol. 60, no. 1, 2 (2011), 171–188.

5. A.H. Ledoan and S.M. Gonek, Zeros of partial sums of the Riemann zeta-function, *Int. Math. Res. Not.*, Vol. 2010, no. 10, 1775–1791.

(d) Synergistic Activities

1. Reviewer: Journal peer review (serving as reviewer in 2007–Present and reviewed over 42 articles in 11 journals); grant review (served as reviewer for National Security Agency Mathematical Sciences Program during 2011–2013); Mathematical Reviews and Zentralblatt MATH (served as reviewer during 2007–2010 and wrote 20 reviews).

2. Organizer: Chattanooga Area Math Circle (serving as Director in 2016-present); American Mathematics Competitions (serving as Manager in 2016-present); Math Kangaroo (served as Co-Manager in 2015); Tennessee Mathematics Teacher's Association High School Math Contest (served as writer for the Precalculus Examination in 2013).

3. Co-organizer: Special Session on Random Processes at AMS 2011 Eastern Sectional Meeting at College of the Holy Cross.

4. Research mentor: Served as research mentor for 10 REU students at UTC during 2013–2015, in addition to 3 graduate student researchers and 2 undergraduate student researchers at UTC since 2014.

5. Program designer: Served on the committee that designed the new concentration Computational and Applied Mathematics for the Ph.D. program in Computational Science.

Yu LIANG, PhD (Computer Science), PhD (Applied Mathematics)
Department of Computer Science and Engineering
University of Tennessee at Chattanooga
615 McCallie Ave., Chattanooga, TN 37403-2598
Tel: 423-425-4351, E-mail: yu-liang@utc.edu or hughliang@gmail.com

A. PROFESSIONAL PREPARATION

• Tsinghua University,	Computer Science	B.S., 1985-1990
• Beijing Polytechnic University	Computer Science	M.S., 1992-1995
• Chinese Academy of Sciences	Computer Science	Ph.D., 1998
• Univ. of Ulster	Applied Mathematics	Ph.D., 2005
• University of Minnesota	Computational Sci.	Postdoc., 2001-2005

B. APPOINTMENT

- 2013-present, Associate Professor / Computer Science**,** University of Tennessee at Chattanooga.
- 2010-2012, Summer Faculty Fellow / Sensor Application, the U.S. Air Force Research Lab.
- 2007-2013, Assistant Professor / Computer Science, Central State University.
- 2006-2007, Visiting Assistant Professor/Computer Science, Embry-Riddle Aeronautical Univ.

C. PUBLICATIONS:

(i) Five most closely related to proposal project

- **Y. Liang**, DL. Wu, D. Huston, G. R. Liu, Y. Li, CL. Gao, J. Ma, Chapter 12: Civil Infrastructure Serviceability Evaluation Based on Big Data, in "Guide to Big Data Application". Edited by S. Srinivasan. Springer Publishing.
- **Y. Liang,** D. Wu, G. Liu, Y. Li, L. Gao, and W. Wu, *Big Data-enabled Multiscale Serviceability Analysis about Aging Bridges*, Elsevier Digital Communications and Networks Journal. August 2016, 97-107. DOI: 10.1016/j.dcan.2016.05.002.
- **Y. Liang** and C. Wu, *A HADOOP-Enabled Sensor-Oriented Information System for Knowledge Discovery about Target-of-interest*, Internet of things - special issue of FUEE Scientific Journal (Impact Factor: 0.460), Vol. 29, No. 3, March 2016, 437-450.
- **Y. Liang,** M. Szularz and L. T. Yang, *Finite-element-wise Domain Decomposition Iterative Solvers Based on Polynomial Preconditioning*, DOI: 10.1016/j.mcm.2012.11.017, Mathematical and Computer Modeling (Impact Factor: 1.346). Vol. 58, Issues 1–2, July 2013, Pages 421-437.
- **Y. Liang**, and Z. Shi, *A Hessian-Free Newton-Raphson Method for the Configuration of Physics Systems Featured by Numerically Asymmetric Force Field*, Mathematical and Computer Simulation, (Impact Factor: 1.109), DOI: 10.1016/j.matcom.2016.11.011 (on press).

(ii) Five other significant publications

- **Y. Liang**, J. Weston and M. Szularz, *Generalized Least-squares Polynomial Preconditioners for Symmetric Indefinite Linear Equations*. Parallel computing (Impact Factor: 1.311), 28(2): 323-341 (2002).
- R. Mohan, Y. Purohit, **Y. Liang**, *Deformation Behavior of Nanoscale Material Systems with Applications to Tensile, Flexural and Crack Propagation*, Journal of Computational and Theoretical Nanoscience (Impact Factor: 0.911), Volume 9, Number 5, May 2012, pp. 649-661(13). **DOI:** 10.1166/jctn.2012.2075.

- J. Zhang, **Y. Liang** and Y. Zhang, *Atomic-level Protein Structure Refinement Using Fragment guided Molecular Dynamics Conformation Sampling*. Structure (Impact factor: 6.347), Vol.19, 1784–1795, December 2011.
- J. Zhang, **Y. Liang**, J.Z. Yan and J. Z. Lou, *Study of the molecular weight dependence of glass transition temperature for amorphous poly (L-lactide) by molecular dynamics simulation*, Polymers (Impact Factor: 3.438), Volume 48, Issue 16, 27 July 2007, 4900-4905.
- **Y. Liang**, S. Li, H. Zhang and C.D. Han, *Timing Sequence Testing for parallel Programs*, Journal of Computer Science and Technology (Impact factor: 0.678), 84-95. Jan. 2000.

D. SYNERGISTIC ACTIVITIES

- Program Committee Member, the 2018 IEEE Big Data Service (March 26-29, 2018. Bamberg, Germany, http://www.big-dataservice.net/)
- Program Committee Member, the 2017 IEEE International Conference on Smart City Innovations (August 4-8, 2017, San Francisco, USA, http://ieee-smartworld.org/2017/sci/).
- Review panelist for the 2015-2017 NSF Graduate Research Fellowship Program (GRFP).
- Editorial Board Member of the International Journal of Security Technology for Smart Device (IJSTSD, URL:http://www.sersc.org/journals/IJSTSD/), Journal of Mathematical Research and Applications (JMRA), and Current Advances in Mathematics (CAM).
- Member of Editorial Board and Program Committee Member, First International Workshop on Security Technology for Smart Device (STSD 2015), URL: http://interworkshop.org/STSD2015.

IV. Biosketches

T. Daniel Loveless
UC Foundation 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: 85 (68 refereed articles/proceedings, 12 non-refereed proceedings, 2 theses, 3 book chapters)

Google Scholar **h-index of 20**; **i10-index of 36**; ≥ 1220 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).

*Recent Conference Proceedings (*Student Author)*

6. *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), Munich, Germany, Oct. 2017.
7. *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.
8. *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.
9. *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. Best student poster award, 37th Annual Government Microcircuit Applications & Critical Technology Conference (GOMACTech), 2012, "Single-Event Hardening Techniques for CMOS Operational Amplifier Design," Raymond W. Blaine, Nicholas M. Atkinson, Jeffrey S. Kauppila, Sarah E. Armstrong, T. Daniel Loveless, W. Timothy Holman, and Lloyd W. Massengill
2. Best poster award, 2011 International Reliability Physics Symposium (IRPS), "Neutron and Alpha Particle Induced Soft-Error Rates for Flip Flops at a 40 nm Technology Node," Srikanth Jagannathan, T. D. Loveless, T. Reece, B. L. Bhuva, S-J. Wen, R. Wong, L. W. Massengill
3. Best paper award, 35th Annual Government Microcircuit Applications & Critical Technology Conference (GOMACTech), 2010, "Recent Advances in Radiation-Hardened-by-Design Analog and Mixed-Signal Circuits," W.T. Holman, L.W. Massengill, B.L. Bhuva, A.F. Witulski, and T.D. Loveless
4. 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
5. Invited speaker for SERESSA (International School on the Effects of Radiation on Embedded Systems for Space Applications), 2009 (Takasaki, Japan), 2010 (São José dos Campos, Brazil), 2011 (Toulouse, France), 2015 (Puebla, Mexico)
6. Conference session chairmanships: 2014 Nuclear and Space Radiation Effects Conference (Single-Event Effects: Devices and ICs), Paris, FR, July 2014, 2012 Single Event Effects Symposium, La Jolla, CA, April 2012

d. Thesis Advisor/Committee Member to (*Total number of students advised: 14)*

Nelson Gaspard, M.S./Ph.D., Vanderbilt University, 2011/2017
Nicholas Atkinson, Ph.D, Vanderbilt University, 2013
Srikanth Jagannathan, Ph.D, Vanderbilt University, 2013
MAJ Raymond Blaine, Ph.D, Vanderbilt University, 2014
Yanran Chen, M.S./Ph.D, Vanderbilt University, 2014/2018
Pierre Maillard, Ph.D, Vanderbilt University, 2014
Trey Reece, Ph.D, Vanderbilt University, 2014
Rachel C. Quinn, M.S., Vanderbilt University, 2014 (*projected Ph.D 2018*)
David McPherson, B.S., University of Tennessee at Chattanooga, 2015
Amee Patel, M.S., University of Tennessee at Chattanooga, (*2017*)
Xiaowen Wang, Ph.D., Vanderbilt University, (*projected 2018*)
Matthew Joplin, M.S., University of Tennessee at Chattanooga, (*projected 2018)*
Ryan Boggs, M.S., University of Tennessee at Chattanooga, (*projected 2019)*
Bharat Patel, M.S., University of Tennessee at Chattanooga, (*projected 2019*)

BIOSKETCH OF THE PI and Co-PIs

Mbakisya A. Onyango: Associate Professor
University of Tennessee at Chattanooga
Department of Civil Engineering
615 McCallie Avenue 2502
Chattanooga, TN 37403
mbakisya-onyango@utc.edu

a. Professional Preparation

Institution	Major(s)	Degree	Year
Kansas State University, USA	Civil/Transportation Eng.	Ph.D.	2009
University of Birmingham, UK	Civil/Highway Eng.	M.Sc.	1995
University of Dar es Salaam, Tz	Civil Engineering	B.Sc.	1992

b. Appointments.

Aug 2016 – Present	UC Foundation Associate Professor, Graduate faculty, Department of Civil Engineering, *University of Tennessee at Chattanooga*. TN
Jan 2010 – 2016:	Assistant Professor, Graduate Faculty, Department of Civil Engineering, *University of Tennessee at Chattanooga*. TN
Aug '09 – Dec '09:	Visiting Assistant Professor, *Kansas State University*, Manhattan, Kansas
Aug '04 – May '09:	Graduate Research and Teaching Assistant, *Kansas State University*, Manhattan, KS.
Jan '01 – July '04:	Deputy Secretary, Information Research and Development, National Council for Technical Education (NACTE), Dar es Salaam, Tanzania
Aug '98 – Dec ' 00:	College Registrar, Technical College Arusha, Tanzania
June '96 – Dec.'00:	Head of Soil, Aggregate and Bitumen Laboratory, Technical College Arusha, Tanzania
June 99 – Dec ' 00	Consulting Senior Materials Engineer, COWI Consult (T) Ltd
Mar. '93 – Dec '00:	Faculty, Technical College Arusha

c. Publications

[1] **Onyango M. A**., Merabti S. A., Owino J. Fomunung I.., Wu W. "Analysis of Cost Effective Pavement Treatment and Budget Optimization for Arterial Roads in the City of Chattanooga" Frontiers of Structural and Civil Engineering Journal, 2017.

[2] **Onyango, M.,** Sen, T., Fomunung I., Owino J. "Evaluation of Treatment Choice, User Cost and Fuel Consumption of Two Roadways in Hamilton County TN Using HDM-4" Journal of Urban Planning and Civil Engineering pp 201 - 218, Edited by Virginia P. Sisiopiku and Ossama E. Ramadan, Published by ATINER, ISBN: 978-960-598-009-2, Athens, Greece, 2015.

[3] Sanford, C., **Onyango, M**.A., Thomas, T.A., Jones, F., and Rollins, B.A. "Evaluation of Cleaning Methods of Pervious Concrete Pavement" Accepted for **ASCE Special publications**. Fairbanks Alaska, August 2015.

[4] Gedafa, D., Hossain, M., Romanoschi, S., **Onyango M**. "Effects of Binder and Mix Properties on the Evolution of Mechanistic Responses of the Accelerated Pavement Testing (APT) Sections" Peer Reviewed conference proceedings, ***Transportation Research Board (TRB) Compendium of Papers,*** Washington D.C., January 2015

[5] **Onyango, M**., Malyuta, D., Owino, J. Chimba, D., "Verification of Pavement Marking Degradation Models using Eastern Tennessee Pavement Marking Retroreflectivity Data" Published by IEEE Special Publication pg 56 - 61, 2014. http://ieeexplore.ieee.org/xpl/articleDetails.jsp?arnumber=7055137.

[5] **Onyango, M.,** Sen, T., Fomunung I., Owino J. "Evaluation of Treatment Choice, User Cost and Fuel Consumption of Two Roadways in Hamilton County TN Using HDM-4" *Peer Reviewed Conference proceedings of the 4th Annual International Conference on Civil Engineering, Structural Engineering and Mechanics*, Athens, Greece, May 2014. **Accepted for publication in the Athens Journal of Technology & Engineering.**

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(a) Professional Preparation

University of District of Columbia, Washington D.C.	Civil Engineering	BS, 1977
Howard University, Washington D.C.	Civil Engineering (Structures)	MS, 1980
Georgia Institute of Technology, Atlanta, Georgia	Civil Engineering (Structures)	Ph.D., 1998

Professional Engineering License – State of Tennessee

(b) Appointments

Sep. 2008 – Present	***Head of Department*** – Department of Civil and Chemical Engineering, UT Chattanooga
Aug. 2015 – Present	***Professor*** - CECS UT Chattanooga
Aug. 2003 – July 2015	***Associate Professor*** - CECS UT Chattanooga
Aug. 1999 – Jul. 2003	***Assistant Professor*** - CECS UT Chattanooga
Jan. 1999 – Mar. 1999	***Adjunct Assistant Professor*** - Georgia Tech, Atlanta, GA
Mar.1995 – Dec. 1998	***Graduate Teaching Assistant*** - Georgia Tech, Atlanta, Georgia
Sep. 1986 – Jul. 1999	***Lecturer*** - Department of Civil Engineering University of Nairobi, Kenya (study leave from July 1992 – May 1997), Head structures group (1988 -1989)
Jul. 1981 – May 1986	***Senior Civil Engineer*** - Shell Oil Inc., New Orleans, Louisiana
Mar. 1981 – Jun. 1983	***Civil Engineer*** - Shell Oil Company, Hoston, Texas
Sep. 1980 – Dec. 1980	***Engineer*** - Electrack Incorporated, Hyattsville, Maryland
Jan. 1980 – Aug. 1980	***Associate Civil Engineer*** - BTML, Falls Church, Virginia.

(c) Publications

1. *Abubakr Ziedan, Ignatius Fomunung**, Joseph Owino**, Melissa Taylor, Andrew Ray.* Is Telecommuting an Effective Travel Demand Management Tool for Mid-Sized Cities? Accepted for presentation and publication at the 22nd International Conference of Hong Kong Society for Transportation Studies – December 2017
2. *Hassan, A., **Owino, J.**, Fomunung, I., Byard, B., Onyango, M., Rollins, B.* "The Impacts of Visual Stability Index on Flowability and Segregation Properties of Self – Consolidating Concrete". Peer Reviewed conference proceedings, *Transportation Research Board (TRB) Compendium of Papers*, Washington D.C., January 2015.
3. *Onyango, M., Sen, T., Fomunung I., **Owino J.*** "Evaluation of Treatment Choice, User Cost and Fuel Consumption of Two Roadways in Hamilton County TN Using HDM-4" *Peer Reviewed Conference proceedings of the 4th Annual International Conference on Civil Engineering, Structural Engineering and Mechanics*, Athens, Greece, May 2014. Accepted for publication in the Athens Journal of Technology & Engineering.
4. *Ignatius Fomunung, **Joseph Owino**, Brent Rollins.* Effects of Wax Emulsion Admixture on Compressive Strength and Surface Characteristics of Roller Compacted Concrete. International Journal of Transportation Technology Transfer in Africa (IJT2A) vol. 1, no. 2, Dec. 2014" edition
5. ***Joseph Owino**, Ignatius Fomunung, Mohammed Khalafala*. The Recent Development in Roller Compacted Concrete. International Journal of Transportation Technology Transfer in Africa (IJT2A) vol. 1, no. 2, Dec. 2014" edition
6. *Ignatius Fomunung, **Joseph Owino**, Mbakisya Onyango, Ammar El Assan.* Evaluation of Two Pavement Rehabilitation techniques for Municipal Roads, ASCE Geotechnical Special Publications Nos 236-243, Proceedings of the Geo-Shanghai International Conference, Shanghai, Edited by Wenqi Ding, Lianyang Zhang, Xiaojun Li, and Xiong Zhang, China, 2014.

7. *Trisha Sen, Mbakisya Onyango,* ***Joseph Owino****, Ignatius Fomunung, Jim Maxwell, Benjamin Byard*. Pavement Management Analysis of Hamilton County Using HDM-4 and HPMA – International Road Federation (IRF) Examiner, Summer 2014

(ii) OTHER SIGNIFICANT PUBLICATIONS

1. *, Mbakisya Onyango, Deo Chimba,* ***Joseph Owino***. "Retrace Pavement Marking Retroreflectivity levels on Tennessee Highways" Tennessee Department of Transportation (TDOT), August 2013 – August 2018.
2. ***Joseph Owino****, Mbakisya Onyango*. "Development of Class P and Class A-SCC (Self-Consolidating Concrete)" Tennessee Department of Transportation (TDOT), June 2013 – June 2015.
3. *Onyango, M., Sen, T., Fomunung I.,* ***Owino J***. "Evaluation of Treatment Choice, User Cost and Fuel Consumption of Two Roadways in Hamilton County TN Using HDM-4" Journal of Urban Planning and Civil Engineering pp 201 - 218*,* Edited by Virginia P. Sisiopiku and Ossama E. Ramadan, Published by ATINER, ISBN: 978-960-598-009-2, Athens, Greece, 2015
4. *Brent Rollins,* ***Joseph Owino****, Ignatius Fomunung,* "All-Hazard Risk Assessment of Critical Transportation Infrastructure in the State of Tennessee" Tennessee Department of Transportation (TDOT), August 2013 – August 2014.
5. *Sen T., Onyango M****., Owino J****., Fomunung I., Byard B*. "Pavement Management Analysis of Hamilton County Using HDM-4 and HPMA – "*International Road Federation (IRF) World Meeting proceedings,* Riyadh Saudi Arabia, November 2013.

(d) Synergistic activities

1. Department Head, Civil and Chemical Engineering, University of Tennessee at Chattanooga, Aug. 2008 - Present.
2. Organizing Chair of the ASEE-SE Conference, University of Tennessee at Chattanooga, April 2-4 2005.
3. National Science Foundation Review Panel EMD Review – July 2003, CCLI ASA Track Review – January 2004, CCLI ASA Track Review – January 2005,CCLI ASA Track Review – January 2006
4. Member (College) – Engineering Assessment Committee, ASEE-SE 2005 Conference Committee, CE Search Committee (03-04), Dean Search Committee (02-03, 03-04), Graduate Committee (01-present); Chair, Petitions committee (02-present), Dean Search Committee (02-03, 03-04)
5. Head-- Civil Engineering's development of assessment processes and tools and new curriculums in support of SACS and ABET.
6. Dean – Student Chapter of the National Society of Black Engineers, (06-Present)
7. Affiliate Professor for Project Lead the Way (PLTW)
8. External Examiner, University of Nairobi (2008 – Present)

(e) Collaborators & other affiliations.

1. Collaborators.

Ignatius Fomunung, Brent Rollins, Neslin Alp, Mbakisya Onyango, Cecelia Wigal, (University of Tennessee at Chattanooga); Mbeche, (University of Nairobi)

2. Thesis Advising.

Mawazo Fortunatus, M.S Student, committee member, Current student
Abubakr Ziedan *M.S. Student*, committee member, graduated 2017
Daniel Malyuta**,** *M.S Student***,** committee member, graduated 2015
Drew Loizeaux**,** *M.S Student***,** committee member, graduated 2015
Saliha Ammour, *M.S Student*, committee member, graduated 2015
Ammar Elhassan *M.S Student*, **Chair**, graduated 2014.
Gloria Neal, *M.S Student*, committee member, graduated 2014
Nick Andrew, *M.S Student*, **Chair**, graduated 2013
Trisha Sen**,** *M.S Student,* committee member, graduated 2013.
Trevor Elliot, *M.S. Student*, **Chair,** graduated, 2008
Mohammad Ali**,** *M.S Student,* **Chair**, graduated 2004
Zain Dwaik, *M.S. Student*, **Chair**, graduated, May 2003

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a. Professional Preparation

- National Institute of Technology, Durgapur, India, Chemical Engineering, B.S., 2008
- The University of Alabama, Tuscaloosa, Alabama, Chemical Engineering, M.S., 2010
- The University of Alabama, Tuscaloosa, Alabama, Chemical Engineering, Ph.D., 2012
- Yale University, New Haven, Connecticut, Chemical Engineering, 2012-2013 (Postdoc.)
- University of South Carolina, Columbia, South Carolina, Arnold School of Public Health, 2013-2014 (Postdoc.)
- The University of Alabama, Tuscaloosa, Alabama, MINT Center, 2014-2015 (Postdoc)

b. Appointments

- Assistant Professor, Department of Civil & Chemical Engineering, August 2017 – present.
- Visiting Assistant Professor, Department of Civil & Chemical Engineering, August 2015- July 2017.

c. Publications (10 out of 32, h-index: 14)

i) Five publications most closely related to proposed project:

- Palchoudhury, S., Zhou, Z., Ramasamy, K., Okirie, F., and Gupta, A., *Self-assembly of P22 protein cages with iron oxide nanoparticles and polyamidoamine dendrimers*. J Mater Res, 2017. 32(2): p. 465
- Palchoudhury, S. and Lead, J. R., A *facile and cost-effective method for separation of oil-water mixtures using polymer-coated iron oxide nanoparticles*. Environ Sci Technol, 2014. 48(24): p. 14558 (communicating author)
- Palchoudhury, S., Xu, Y., Rushdie, A., Holler, R., and Bao, Y., *Controlled synthesis of iron oxide nanoplates and nanoflowers.* Chem Commun, 2012. 48(85): p. 10499.
- Palchoudhury, S., Xu, Y., Goodwin, J., and Bao, Y., *Synthesis of multiple platinum attached iron oxide nanoparticles.* J Mater Chem, 2011. 21(11): p. 3966.
- Palchoudhury, S., An, W., Xu, Y., Qin, Y., Zhang, Z., Chopra, N., Holler, R., Turner, C. H., and Bao, Y., *Synthesis and growth mechanism of iron oxide nanowhiskers.* Nano Lett, 2011. 11(3): p. 1141.

ii) Five other significant publications:

- Zhou, Z., Bedwell, G. J., Li, R., Palchoudhury, Prevelige, P. E., and Gupta, A., *Pathways for gold nucleation and growth over protein cages.* Langmuir, 2017. 33(23): p. 5925.
- Negi, D. S., Sharona, H., Bhat, U., Palchoudhury, S., Gupta, A., and Datta, R., *Surface spin canting in Fe_3O_4 and $CoFe_2O_4$ nanoparticles probed by high-resolution electron energy loss spectroscopy.* Phys Rev B: Condens Matter, 2017. 95(17): p. 174444.
- Zhang, C.; Wang, Z.; Bhoyate, S.; Morey, T.; Neria, B.; Vasiraju, B.; Gupta, G.; Palchoudhury, S.; Kahol, P.K.; Mishra, S.R.; Perez, F.; Gupta, R., *MoS_2 decorated carbon nanofibers as efficient and durable electrocatalyst for hydrogen evolution reaction.* C, 2017. 3(4): p. 33 (Featured as cover art)
- Palchoudhury, S., Ramasamy, R., and Gupta, A., *Recent progress in spintronic materials.* Material Matter, 2016. 11(4): p. 97 (Invited Paper).
- Ghosh, A., Palchoudhury, S., Thangavel, R., Zhou, Z., Naghibolashrafi, N., Ramasamy, K., and 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.* Chem Commun, 2016. 52(2): p. 264

d. Synergistic Activities

- Submitted proposal for **ORAU's Ralph E. Powe Junior Faculty Enhancement Award** 2018, "A new class of penternary chalcogenide nanocrystals and thin films for solar energy conversion applications ($10,000); proposal has been selected through UTC's internal competition.

- **CINT User Proposal award, Sandia National Lab** # 2017BU0060, "Understanding the effect of engineered nanoparticles in agriculture." This award allows me to use the transmission electron microscope at Sandia National Lab for characterizing our new bio-inspired materials.

- **CINT User Proposal award, Sandia National Lab** #2016BU0031, "Developing a new family of wurtzite $CuZn_2ASe_4$ (A=Al, Ga, In) nanocrystals for solar cell application." I received this award to use the electron microscopes and other material characterization facilities at Sandia National Lab for analyzing the new nanomaterials synthesized in my lab at UTC.

- **THEC Center for Excellence in Applied Computational Science & Engineering award** #R041302234: I have an established background in mentoring undergraduate and graduate students in interdisciplinary research. I am a recipient of the THEC CEACSE award ($89,211) for my interdisciplinary project combining computational and experimental methods to analyze nanoparticle transport titled "Computational Fluid Dynamic Approach to Predict Transport and Distribution of Nanodrugs".

- **Editorial board member and reviewer**: I am the editorial board member for the International Journal of Measurement Technologies and Instrumentation Engineering. I am a reviewer for several high-impact nanotechnology journals like J Appl Phys, Langmuir, Appl Phys Lett, Nanoscale, Inorg Chem, and Environ Sci Technol. I have also reviewed book chapters for IGI Global and Cengage. I am currently serving as the chief editor for a special issue for the journal of Nanomaterials.

- **Research Highlights**: My work on engineering a new phase transfer technique to form water-soluble iron oxide nanoparticles has been highlighted in ***Nature***, "Chemistry: Iron nanoparticles into blood." Nature 2011, 476, 9. "A new family of wurtzite-phase Cu_2ZnAS_{4-x} and $CuZn_2AS_4$ (A= Al, Ga, In) nanocrystals for solar energy conversion applications", Chem Commun 2016, 52, 217 has featured as the cover art. "MoS_2 decorated carbon nanofibers as efficient and durable electrocatalyst for hydrogen evolution reaction" has featured as the top cover of the journal C 2017, 3(4).

- **Invited Lecture**: I have presented an invited lecture on different applications of hybrid nanoparticles at the International Conference and Exhibition on Materials Science and Engineering held in Atlanta on Sep 2016, "Synthesis and Characterization of Hybrid Nanoparticles for Biomedical and Environmental Remediation Applications".

- **Tennessee Board of Architectural and Engineering Examiners laboratory equipment award,** #R041320005: I have been a co-PI for the $26,761 development grant awarded for undergraduate chemical engineering laboratories. I have started developing a fully equipped nano lab station with this award.

- **Mentees**: 11 undergraduate students and 4 graduate researchers; graduated 1 M.S. Thesis student in 2016; full tuition for 2 graduate students and partial tuition for 1 graduate student, hourly pay for 3 graduate students and 4 undergraduate students were supported from my THEC-CEACSE grant in Fall 2017 and Spring 2018.

Jared A. Pienkos
Assistant Professor
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Jared.pienkos@furman.edu

(a) Professional Preparation

Hamilton College	Clinton, NY	Chemistry and Mathematics	B.A. 2009
University of Virginia	Charlottesville, VA	Chemistry	Ph.D. 2014
Furman University	Greenville, SC	Inorganic Photophysics	Postdoc, 2014-2018

(b) Appointments

University of Tennessee Chattanooga
Assistant Professor, Department of Chemistry 2018-present

(c) Publications

Vieira, N. C.; Pienkos, J. A.; McMillen, C. D.; Myers, A. R.; Clay, A. P., Wagenknecht, P. S. A trans-bidentate bis-pyridinyl ligand with a transition metal hinge. *Dalton Transactions* **2017**, 46, 15195.

Pienkos, J. A.; Agakidou, A. D.; Trindle, C. O.; Herwald, D. W.; Altun, Z.; Wagenknecht, P. S. Titanocene as a New Acceptor (A) for Arylamine Donors (D) in D−π–A Chromophores. *Organometallics* **2016**, 35, 2575.

Turlington, M. D.; Pienkos, J. A.; Carlton, E. S.; Wroblewski, K. N.; Myers, A. R.; Rack, J. J.; Wagenknecht, P. S. Complexes with Tunable Intramolecular Ferrocene to Ti^{IV} Electronic Transitions: Models for Solid State Fe^{II} to Ti^{IV} Charge Transfer. *Inorg. Chem.* **2016**, 55, 2200.

Macleod, B. L.; Pienkos, J. A.; Wilson, K. B.; Sabat, M.; Myers, W. H.; Harman, W. D. Synthesis of Novel Hexahydroindoles from the Dearomatization of Indoline. *Organometallics*. **2016**, 35, 370.

Lankaenau, A. W.; Iovan, D. A.; Pienkos, J. A.; Salomon, R. J.; Wang, S.; Harrison, D. P.; Myers, W. H.; Harman. W. D. Enantioenrichment of a Tungsten Dearomatization Agent Utilizing Chiral Acids. *JACS* **2015**, 137, 3649.

Pienkos, J. A.; Kinsely, A. T.; Liebov, B. K.; Teran, V.; Zottig, V. E.; Sabat, M.; Myers. W. H.; Harman. W. D. Tungsten-Mediated Selective Ring Opening of Vinylcyclopropanes. *Organometallics* **2014**, 33, 267.

MacLeod, B. L.; Pienkos, J. A.; Myers, J. T.; Sabat, M.; Myers, W. H.; Harman. W. D. Stereoselective Synthesis of trans-Tetrahydroindolines Promoted by a Tungsten π Base. *Organometallics* **2014**, 33, 6286.

Myers, J. T.; Shivokevich, P. J.; Pienkos, J. A.; Myers, W. H.; Harman, W. D. Synthesis of 2-Substituted 1,2-Dihydronaphthalenes and 1,2-Dihydroanthracenes Using a Recyclable Molybdenum Dearomatization Agent. *Organometallics* **2015**, 34, 3648.

Shivokevich, P.; Myers, J.; Smith, Jacob; Pienkos, J.; Dakermanji, S.; Pert, E.; Welch, K.; Trindle, C.; Harman, W. D. Enantioenriched Molybdenum Dearomatization: Dissociative Substitution with Configurational Stability. *Organometallics* **2018**, *ASAP*.

Pienkos, J. A.; Zottig, V. E.; Iovan, D. A.; Li, M.; Harrison, D. P.; Sabat, M.; Salomon, R. J.; Strausberg, L.; Teran, V. A.; Myers, W. H.; Harman, W. D. Friedel–Crafts Ring-Coupling Reactions Promoted by Tungsten Dearomatization Agent. *Organometallics* **2013**, 32, 691.

(d) Synergistic Activities

- Helped organize science workshops for local high school students and teachers (2015-present).
- Organized three guest lectures at Furman University (2016-2017)
- Organized two guest lectures at University of Virginia (2012-2013)
- University of Virginia Chemistry Graduate Student Council (2010-2013)

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Department of Biology, Geology & Environmental Science, SimCenter
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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 in Department of Computer Science & Engineering and Department of Biology, Geology & Environmental Science, and SimCenter, August 2016 – present.
- Associate Professor, Department of Biology, Spelman College, September 2015 – July 2016.
- Assistant Professor, Department of Biology, Spelman College, August 2009 – August 2015.
- Assistant Professor, Department of Agricultural and Environmental Sciences, and Department 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.** Dr. 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/. Dr. Qin leads the Health and Biosystems program at the 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." Dr. Qin is the recipient of an NSF CAREER award for his research on mathematical modeling of cellular aging and development of computational tools for studies on aging.

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

- **Quantitative Biology Community**: Dr. 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). Dr. Qin also recently co-organized the 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. Dr. 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. Dr. 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," and "PCR product analysis followed by restriction enzyme analysis, ApE."

- **Open Science and Reproducible Research**, https://github.com/hongqin and https://github.com/QinLab. Dr. Qin is active in the open science community and support reproducible research initiative. Dr. Qin and members in his research group have been publicly 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. Bharat Patel*, Matthew Joplin*, Ryan Boggs*, Donald Reising, , Lloyd Massengill, T. Daniel Loveless, "Ionizing Radiation Effects Spectroscopy (IRES) for Analysis of Total-Ionizing Dose Degradation in Voltage-Controlled Oscillators ," IEEE Nuclear & Space Radiation Effects Conference (NSREC) 2018, UNDER REVIEW.
2. Charles G. Wheeler* and Donald R. 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.
3. Donald R. Reising, Michael A. Temple, and Julie M. 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.
4. Donald R. Reising, David A. Prentice, and Michael A. Temple, "An FPGA Implementation of Real-Time RF-DNA Fingerprinting for RFINT Applications." 2011 Military Communications Conference (MILCOM 2011), Oct. 2011.

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

1. Mohammed Fadul*, Amee Patel*, Donald Reising, T. Daniel Loveless, and Mina Sartipi, "Estimating Energy Consumption Using Instantaneous Temperature", 2018 ASHRAE Conference, ACCEPTED.
2. Paul K. Harmer, Donald R. Reising, and Michael A. Temple, "Classifier Selection for Physical Layer Security Augmentation in Cognitive Radio Networks". IEEE Int'l Conference on Communications (ICC), Jun. 2013.
3. Donald R. Reising, and Michael A. Temple, "WiMAX Mobile Subscriber Verification Using Gabor-Based RF-DNA Fingerprints," IEEE Int'l Conference on Communications (ICC), Jun. 2012.
4. Donald R. Reising, Michael A. Temple, and Mark E. 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.

5. McKay D. Williams, Michael A. Temple, and Donald R. Reising, "Augmenting Bit-Level Network Security Using Physical Layer RF-DNA Fingerprinting," IEEE Global Communications Conference (GLOBECOM), Dec. 2010.

d. Synergistic Activities

7. 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.
8. Faculty advisor for the Electrical Engineering Department Senior Design Course, 2015-present.
9. Principle Investigator for project titled, "An Analysis of Power Quality Waveforms for Greater Grid Reliability". This project is funded through the Electrical Power Research Initiative (EPRI) Distribution Modernization Demonstration (DMD) Data Mining Initiative from August 2017 through May 2019. The focus of this project is the development of a visualization process to be used by power industry engineers for electrical disturbance analysis. This visualization process will target nine specific and previously identified electrical disturbance types.
10. Faculty lead and coordinator for University of Tennessee at Chattanooga's College of Engineering and Computer Science MakerSpace. The MakerSpace provides an environment and equipment to nurture and facilitate entrepreneurial as well as creative endeavors of UTC's undergraduate and graduate students, 2015-Present.
11. Completed Electric Power Board's (EPB) Engineering Scholars course in June of 2015. This teaches engineers and researchers the processes, equipment, policies, company organization, and challenges of EPB. The purpose of this course is to establish a basic knowledge of EPB's inner workings to facilitate collaborative work.

ARUNA SARAM
3491 Lamuel Field Ln High Point NC 27265

Summary:

- Proficient in SAS/BASE, SAS/SQL, SAS/Macro, SAS/Connect, SAS/Access, SAS/ODS, SAS/STAT and SAS/GRAPH, SAS/IML, SAS Enterprise Guide, R
- Data preparation for various statistical modeling which includes data cleaning, descriptive analysis, missing data analysis, data validations, and data triangulations
- Strong experience in coding using SQL, Procedures/Functions, SAS macros
- Hands on experience in using different Statistical tools such as SAS, IBM SPSS, Minitab, R
- Excellent command in writing complex routines for Data Validations, Data Extraction, transformation and loading to target decision support systems using MS Excel, Pivot tables and SAS on various environments.
- Proven skills in Data Cleansing, Data Archival, Data Migration, ad-hoc reporting and coding utilizing SAS on UNIX, Windows

EDUCATION & CREDENTIALS

- **Ph.D. in Computational Science with concentration in Computational & Applied Mathematics (GPA 4.0) -**The University of Tennessee at Chattanooga, Chattanooga, TN, USA - Currently in the Program
- **M.Sc. in Statistics (GPA 3.65) –** Sam Houston State University, Houston, Texas, USA - 2006
- **MBA in Actuarial Science (GPA 3.18)** – St. John's University, New York, USA - 2000
- **B.Sc. in Mathematics (GPA 3.02)–** University of Colombo, Sri Lanka - 1995

HONORS

- **Dean scholarship from College of Arts and Sciences - Sam Houston State University, Texas, USA**
- **Superior Achievement in The field of Mathematics - National Honorary Mathematics Society, Texas, USA**

PROFESSIONAL EXPERIENCE

- **Graduate Research Assistant - The University of Tennessee at Chattanooga, TN, USA**
  January 2018 – Present
- **Statistical Analyst/Statistician - Addon Technologies, Livonia MI, USA**
- **October 2016 – July 2017**
- **Statistical Analyst/Statistician - GroundsTech Consulting, Burnaby BC, Canada**
  September 2012 – September 2016
- **Client – Vancouver Real Estate Board, ENMAX, CIBC**

- **Research Assistant - Lethbridge University – Lethbridge AB**
  May 2009 – September 2012
-

- **Statistical Analyst/SAS Programmer - Gunasekera & Co., Anuradapura, Sri Lanka**
  September 2007 - April 2009

- **Graduate Teaching & Research Assistant - Sam Houston State University, TX, USA**
  May 2004 – August 2007

TECHNICAL SKILLS

SAS Tools:	SAS/BASE, SAS/Macros, SAS/STAT, SAS/ETS, SAS/Access, SAS/AF, SAS/IML, SAS/SQL, SAS AF Frame, SAS Enterprise Guide, SAS Web Report Studio, SAS Enterprise Miner
Programming	SAS, R, Matlab, Visual Basic SQL, PL/SQL, Teradata, and Unix
DBMS:	Oracle 11g/10g/9i, SQL Server, Microsoft Access, ArcGIS Server
Operating Systems:	Unix, Windows 3.1, Win NT 4.0, Windows 2000/XP/7, MS-DOS
MS Office suite	MS word, MS PowerPoint, MS Excel

CONFERENCES

- **Testing Outliers Using a Mixture Population** (Presentation and Published at ASA)
  Joint Statistical Meeting - Seattle, USA – 2006

- **Taguchi Approach to the Design of Experiment for Quality and Cost** (Presentation)
  Mathematical Association of America, Midwestern State University in Texas, April 6-8, 2006

Mina Sartipi, PhD

UC Foundation Professor - Department of Computer Science and Engineering
Lead Scientist for Smart Cities and Urban Science
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 **Lead Scientist Smart City and Urban Systems**
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] J. Cho, Z. Hu, and M. Sartipi, "Non-Intrusive A/C Load Disaggregation Using Deep Learning," accepted to appear in the Proc. of 2018 IEEE Power & Energy Society T&D Conference & Exposition, April 2018.

[2] J. Cho, Z. Hu, and M. Sartipi, "A/C Load Forecasting Using Deep Learning," in the Proc. of IEEE CPS - Big Data and Data Science, December 2017.

[3] 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.

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

[5] R. Thompson, Z. Hu, J. Cho, J. Stovall, A. Harris, and M. Sartipi, "Enhancing Driver Awareness Using See-Through Technology." accepted WCX17: SAE World Congress Experience, 2018.

Other Significant Products

[1] R. Thompson, Z. Hu, J. Cho, J. Stovall, A. Harris, and M. Sartipi, "See-Through Technology Using V2X Communication," in the Proc. of ACM Mid-Southeast, November 2017.

[2] A. Harris, H. True, Z. Hu, J. Cho, N. Fell, and M. Sartipi, "Fall Recognition using Wearable Technologies and Machine Learning Algorithms," the Proc. of IEEE Big Data Conference, December 2016.
[3] M. Sartipi, "On the Rate-Distortion Performance of Compressive Sensing in Wireless Sensor Networks", in Proc. of International Conference on Computing, Networking and Communications, January 2013.
[4] J. Cho, Z. Hu, N. Fell, G. Heath, R. Qayyum, and M. Sartipi, "Hospital Discharge Disposition of Stroke Patients in the State of Tennessee," Journal of the Southern Medical Association, accepted, September 2017.
[5] J. Cho, Z. Hu, and M. Sartipi, "Post-stroke Discharge Disposition Prediction using Deep Learning," in Proc. of IEEE SoutheastCon, March 2017.

D. Synergistic Activities

- **IEEE Senior Member**
- **Founding Director**
  2012-present, Smart Communications and Analysis Lab
- **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

Joey Shaw
UC Foundation Professor
Department of Biology, Geology, Environmental Science
University of Tennessee at Chattanooga

a. Professional Preparation

University of Tennessee, Knoxville	Botany	Ph.D., 2005
University of Tennessee, Knoxville	Botany	M.S., 2001
University of Tennessee at Chattanooga	Biology	B.S., 1998

b. Appointments

2015 – 2018: Full Professor and Curator of the UTC herbarium collection, Department of Biological and Environmental Sciences, The University of Tennessee at Chattanooga
2010 – 2015: Associate Professor and Curator of the UTC herbarium collection, Department of Biological and Environmental Sciences, The University of Tennessee at Chattanooga
2005 – 2010: Assistant Professor and Curator of the UTC herbarium collection, Department of Biological and Environmental Sciences, The University of Tennessee at Chattanooga
2004 – 2005: Yates Fellow, University of Tennessee, Knoxville
2004 – 2005: Holleander Fellow, University of Tennessee, Knoxville
1998 – 2004: Graduate Teaching Assistant, Dept. of Botany, University of Tennessee, Knoxville

c. Products

Five products relevant products

*Indicates undergraduate authors, **indicates graduate student authors

1. Nelson, G. P. Sweeney, L.E. Wallace, R.K. Rabeler, D. Allard, H. Brown, J.R. Carter, M.W. Denslow, E.R. Ellwood, C. Germain-Aubrey, E. GIlbert, E. Gillespie, L.R. GOertzen, B. Legler, D.B. Marchant, T.D. Marsico, A.B. Morris, Z. Murrell, M. Nazaire, C. Neefus, S. Oberreiter, D. Paul, B.R. Ruhfel, T. Sasek, J. Shaw, P.S. Soltis, K. Watson, A. Weeks, and A.R. Mast. 2015. Digitization workflows for flat sheet and packets of Plants, Algae, and Fungi. *Applications in Plant Sciences.* 3: 1500065.
2. Tennessee Flora Committee. 2015. Guide to the Vascular Plants of Tennessee (editors: E.W. CHESTER, B.E. WOFFORD, J. SHAW, D. ESTES, AND D. WEBB [RANKED IN ORDER OF CONTRIBUTION]). University of Tennessee Press, Knoxville, Tennessee.
3. *Blyveis, E., and J. Shaw. 2012. The vascular flora and phytogeographical analysis of the Tennessee River Gorge, Hamilton and Marion counties, Tennessee. *Southeastern Naturalist* 11: 599-636.
4. Beck, J., C. Ferguson, M. Mayfield, and J. Shaw. 2014. Reduced population genetic variation in black cherry (*Prunus serotina* subsp. *serotina*, Rosaceae) at its western range limit in Kansas. *Northeastern Naturalist* 21:472-478.**Huskins, S. and J. Shaw. 2010. The vascular flora of North Chickamauga Creek Gorge State Natural Area, Hamilton and Sequatchie Counties, Tennessee. *Castanea* 75:101-125.
5. Shaw, J., E. Lickey, E. E. Schilling, and R. Small. 2007. Comparison of whole chloroplast genome sequences to choose noncoding regions for phylogenetic studies in angiosperms: The tortoise and the hare III. *American Journal of Botany* 94: 275-288.

Other significant products

*Indicates undergraduate authors, **indicates graduate student authors

1. Shaw, J. **H. Shafer, *O.R. Leonard, M.J. Kovach, M. Schorr, and A.B. Morris. 2014. Chloroplast DNA sequence utility for the lowest phylogenetic and phylogeographic inferences in angiosperms: Tortoise and Hare IV. *American Journal of Botany* 101: 1987-2004.
2. Beck, J., C. Ferguson, M. Mayfield, and J. Shaw. 2014. Reduced population genetic variation in black cherry (*Prunus serotina* subsp. *serotina*, Rosaceae) at its western range limit in Kansas. *Northeastern Naturalist* 21:472-478.
3. Anderson, T.M., J. Shaw, and H. Olff. 2011. Ecology's cruel dilemma, phylogenetic trait evolution and the assembly of Serengeti plant communities. *Journal of Ecology* 99: 797-806.
4. *Montgomery, M., and J. Shaw. 2012. *Clematis fremontii* in the southeastern United States, naturally occurring relicts or recently introduced populations? *Tipularia* 27: 11-18.
5. **Miller, R.J., A. Carroll, T.P. Wilson, and J. Shaw. 2009. Spatiotemporal analysis of three common wetland invasive plant species using herbarium specimens and geographic information systems. *Castanea* 74: 133-145.

d. Synergistic Activities (selected, past five years):

1. With Ashley Morris and Dwayne Estes founded the Tennessee Herbarium Consortium (THC - https://www.facebook.com/tnherbariumconsortium/) to unite Tennessee Curators and provide connectivity between faculty curators.
2. Leading an effort with Ashley Morris, Dwayne Estes, and Brad Ruhfel (Eastern Kentucky University) to use SERNEC data to build a Tennessee-Kentucky Plant Atlas (http://www.plantatlas.usf.edu) (funding already secured from Tennessee native Plant Society and Kentucky Native Plant Society and contracts in place with University of South Florida).
3. Organized and led multi-university herbarium digitization kickoff blitzes at Rhodes College and the University of Tennessee at Martin. Also, I have two scheduled for the next few months (University of the South, August 11 and East Tennessee State University, September 10).
4. Direction of undergraduate and graduate (12 MS students) student research in areas of floristic botany, vascular plant taxonomy and systematics, community ecology, and invasive species ecology. As part of their projects, all were trained in proper methods of specimen collection, processing, data collection, and curatorial aspects associated with preserving and maintaining collections.
5. Secretary for the Tennessee Flora Committee, 2005-present; this committee has produced the *Fifth Checklist of Tennessee Vascular Plants* and the *Guide to the Vascular Flora of Tennessee*.

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. Hereth, E., Sreenivas, K., Taylor, L.K., and Nichols, D.S., "An Automatic Parallel Octree Grid Generation Software with an Extensible Solver Framework and a Focus on Urban Simulation" AIAA Paper 2017-0587, Grapevine, TX, January 2017.
2. 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.
3. 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.

4. Mittal, A., Briley, W.R., Sreenivas, K., and Taylor, L.K., "A Parabolic Velocity-Decomposition Method for Wind Turbines," Journal of Computational Physics Vol. 330, pp 650–667, 2017.
5. 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.

D. 5 Other Significant Publications:

1. Sreenivas, K., Mittal, A., Hereth, L., and Taylor, L.K., "Computational Simulation of the Interaction Between Tandem Wind Turbines with Offset," *AIAA Paper 2015-0224*, 33rd Wind Energy Symposium, AIAA SciTech 2015.
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.

E. 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)
- SimCenter leadership role in high-performance cluster computing, including cluster design, benchmarking, acquisition, and resource allocation (University of Tennessee at Chattanooga)
- Thesis Advisor for 5 Ph.D. and 7 M.S. students (University of Tennessee at Chattanooga)
- Committee Member for 7 Ph.D. students, 4 M.S. students, and mentor for 2 Undergraduate Student Researchers (University of Tennessee at Chattanooga)
- Thesis Advisor for 2 MS Students and committee member for 3 MS and 1 Ph.D. student (Mississippi State University)

F. 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

Craig R. Tanis

Professional Preparation

Tulane University	Computer Engineering / Robotics	BSE	1997
Tulane University	Computer Science	MS	1998
University of Tennessee	Computational Engineering	Ph.D.	2013

Appointments

- **2014-Present:** Assistant Professor, Faculty of Computer Science, University of Tennessee at Chattanooga
- **2010-2013:** Lecturer, Faculty of Computer Science, University of Tennessee at Chattanooga
- **2007-2010:** Graduate Student Researcher, SimCenter: National Center for Computational Engineering, University of Tennessee at Chattanooga
- **1999-2006**: Senior Programmer, Advance Internet, Jersey City, NJ
- **1996-1998**: Graduate Student Researcher, Mobile Robotics, Tulane University

Five Products Most Relevant to Proposal

1. R. Whalen, Y. Huang, C. Tanis, A. Sawant, B. Uzzi, and N. Contractor, "Citation Distance: Measuring Changes in Scientific Search Strategies," Proceedings of ACMWWW 2016, BigScholar.
2. W. K. Anderson, L. Wang, S. Kapadia, C. Tanis, and B. Hilbert, "Petrov-Galerkin and discontinuous-Galerkin methods for time-domain and frequency-domain electromagnetic simulations," Journal of Computational Physics, vol. 230, no. 23, pp. 8360–8385, Sep. 2011.
3. C. Tanis, "A NEW SOFTWARE FRAMEWORK FOR UNSTRUCTURED MESH REPRESENTATION AND MANIPULATION," University of Tennessee at Chattanooga, 2013.
4. C. Tanis, Splatter (2013-Present). Public git repository: `https://bitbucket.org/ctanis/splatt`.

Synergistic Activities

1. XSEDE Campus Champion for University of Tennessee at Chattanooga, 2014-Present
2. XSEDE Campus Champion Fellow 2015-16
3. Course developer for two graduate-level courses: (1) High-Performance Computing; (2) Parallel programming
4. Departmental "Teacher of the Year" 2011, 2012, 2013, 2014

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

Publications

Related Publications

1. C. Yang and **J. Wang**, On the intrinsic dynamics of bacteria in waterborne infections, *Mathematical Biosciences*, vol. 296, pp. 71-81, 2018.

2. C. Yang, X. Wang, D. Gao and **J. Wang**, Impact of awareness programs on cholera dynamics: Two modeling approaches, *Bulletin of Mathematical Biology*, vol. 79, pp. 2109-2131, 2017.

3. X. Wang, D. Posny and **J. Wang**, A reaction-convection-diffusion model for cholera spatial dynamics, *Discrete and Continuous Dynamical Systems B*, vol. 21, pp. 2785-2809, 2016.

4. X. Wang, D. Gao and **J. Wang**, Influence of human behavior on cholera dynamics, *Mathematical Biosciences*, vol. 267, pp. 41-52, 2015.

5. D. Posny and **J. Wang**, Modeling cholera in periodic environments, *Journal of Biological Dynamics*, vol. 8(1), pp. 1-19, 2014.

Other Publications

1. D. He, X. Wang, D. Gao and **J. Wang**, Modeling the 2016-2017 Yemen cholera outbreak with the impact of limited medical resources, 2018. Under review.

2. L. Cai, C. Modnak and **J. Wang**, An age-structured model for cholera control with vaccination, *Applied Mathematics and Computation*, vol. 299, pp. 127-140, 2017.

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

4. D. Posny and **J. Wang**, Computing basic reproductive numbers for epidemiological models in nonhomogeneous environments, *Applied Mathematics and Computation*, vol. 242, pp. 473-490, 2014.

5. Z. Mukandavire, S. Liao, **J. Wang**, H. Gaff, D. Smith, and J. Morris, Estimating the reproductive numbers for the 2008-2009 cholera outbreaks in Zimbabwe, *Proceedings of the National Academy of Sciences*, vol. 108, pp. 8767-8772, 2011.

Synergistic Activities

- Reviewer: *Journal peer review (more than 60 manuscripts in 37 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).*

- Organizer: *Minisymposium on "Simulation and Analysis in Biological Systems", the 35th SIAM-SEAS Conference, Charlotte, NC, March 2011; Minisymposium on "Recent Advances in Mathematical Epidemiology and Ecology", The 4th International Conference on Mathematical Modeling and Analysis, Lubbock, TX, October 2013; International Conference on "Recent Advances in Linear Algebra and Graph Theory", Chattanooga, TN, March 2016; Interdisciplinary Mathematics Summer Camp for High School Students, Chattanooga, TN, 2016 - ; Workshop on "Epidemic Dynamics of Cholera in Non-homogeneous Environments", American Institute of Mathematics, San Jose, CA, July 2016.*

- Grant activity: *Nearly 2.5 million of research 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, 2018), Faculty Search Committee (2009, 2010, 2014, 2015, 2016, 2017, 2018), Tenure and Promotion Committee (2015, 2016, 2017, 2018), Computational Science Ph.D. Screening Committee (2016, 2017), 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; Trimble 2018), Qualifying Examination Committees (Li, Posny, Phuworawong, 2011; Malali, 2012; Ghazizadeh, 2013; Trimble, 2017).*

- Honors and awards: *UNUM Chair of Excellence in Applied Math (2014 -); College of Arts & Sciences Outstanding Research Award (2018); College of Arts & Sciences Dean's Award (2016); Sigma Xi (2009); Faculty Innovator Award (2009); Inclusion in Who's Who in America (2008); Distinguished Graduate Teaching Associate Award (2004).*

31 January 2018

Robert S. Webster, Ph.D.

Office: (423) 425-5509
E-Mail: Robert-Webster@utc.edu

Education

Ph.D., Aerospace Engineering, Mississippi State University, May, 2001
M.S., Aerospace Engineering, Mississippi State University, August, 1994
Bachelor of Aerospace Engineering, Auburn University, December, 1986

Employment

Associate Professor, Department of Mechanical Engineering, University of Tennessee at Chattanooga, January, 2017 to Present
Associate Research Professor, Department of Computational Engineering, University of Tennessee at Chattanooga, July, 2008 to December, 2016
Assistant Research Professor, Department of Computational Engineering, University of Tennessee at Chattanooga, December, 2002 to July, 2008
Postdoctoral Fellow, Engineering Research Center, Mississippi State University, May, 2001 to December, 2002
Graduate Research Assistant (PhD Program), Engineering Research Center, Mississippi State University, August, 1994 to May, 2001
Graduate Research Assistant (MS Program), Engineering Research Center, Mississippi State University, January, 1992 to August, 1994
Aerospace Technologist, NASA Marshall Space Flight Center (MSFC), January, 1989 to December, 1991
Mechanical Engineer, US Army TMDE Support Group, Redstone Arsenal, AL, January, 1987 to December, 1988

University Service

Major Professor for 1 Master Degree and 1 Doctoral Degree Candidates
Committee Member for 5 Master Degree and 2 Doctoral Degree Candidates
Member of ME Departmental Undergraduate Curriculum Committee
Member of ME Departmental Strategic Planning Committee
Member of University Undergraduate Curriculum Committee

Courses Taught

ENGR-1030, Basic Engineering Science; calculus-based Newtonian mechanics
ENCM-7340, Viscous Flow Computation; computation of viscous flow fields, introduction to turbulent flows and turbulence modeling
ENCH-3320, Heat Transfer Processes; introduction to heat transfer in solids and fluids
ENME-3090, Heat and Mass Transfer; introduction to heat transfer in solids and fluids

Professional Affiliations and Honors

AIAA Inlets, Nozzles, and Propulsion Systems Integration Technical Committee; elected 2017
AIAA Gas Turbine Engine Technical Committee; 2008 – 2015; Member (presently Emeritus Member)
American Society of Mechanical Engineers (ASME); 2001 – Present; Member
American Institute of Aeronautics and Astronautics (AIAA); 1995 – Present; Senior Member
Sigma Gamma Tau (Aerospace Engineering Honor Society); Auburn University, 1986

Awards

AIAA Best Paper in Air Breathing Propulsion, 2005/2006; awarded by AIAA Air Breathing Propulsion Technical Committee for *AIAA-2006-0418* (co-author) entitled "Numerical Simulation of Stall and Stall Control in Axial and Radial Compressors"; awarded at 42nd AIAA/ASME/SAE/ASEE Joint Propulsion Conference Awards Luncheon, 12 July, 2006.

Reviewer

ASME TURBO EXPO: 2004 – 2005, 2009 – 2018
AIAA Journal: 2010, 2013, 2017
AIAA Aerospace Sciences Meeting: 2010, 2015, 2018
AIAA Aviation Forum: 2018
International Journal for Computational Methods in Engineering Science & Mechanics: 2010
U.S. Army Research Office Grant Review: 2011
Aerospace Science and Technology: 2012
AIAA Joint Propulsion Conference: 2013 – 2018
AIAA Journal of Propulsion and Power: 2014 – 2015
AIAA Journal of Aircraft: 2015
Engineering Science and Technology, an International Journal: 2015
ASCE Journal of Aerospace Engineering: 2016-2017

Publications

1. Tanis, C., Sreenivas, K, Newman, J. C. and Webster, R. S., "Performance Portability of a Multiphysics Finite Element Code," Submitted to the 2018 AIAA AVIATION Forum (Accepted for Presentation/Publication)
2. Sreenivas, K., Webster, R. S., and Hereth, E. A., "Impact of High-Order Spatial Accuracy on Multi-Stage Turbomachinery Simulations," *AIAA-2017-4823*, 53rd AIAA/SAE/ASEE Joint Propulsion Conference, July, 2017.
3. Sreenivas, K, Webster, R. S., Hereth, E. A., Berdanier, R. A., and Key, N. L., "Computational Simulations of a Multi-stage Subsonic Research Compressor," *AIAA-2016-0395*, 54th AIAA Aerospace Sciences Meeting, January, 2016.
4. Webster, R. S., Sreenivas, K., Hyams, D. G., Hilbert, C. B., Briley, W. R., and Whitfield, D. L., "Demonstration of Sub-system Level Simulations: A Coupled Inlet and Turbofan Stage," *AIAA-2012-4282*, 48th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, August, 2012.
5. Chen, J-P, Webster, R. S., Hathaway, M. D., Herrick, G. P., and Skoch, G. J., "Numerical Simulation of Stall and Stall Control in Axial and Radial Compressors," *AIAA-2006-0418*, 44th AIAA Aerospace Sciences Meeting, January, 2006.

Participation in Grants/Contracts

1. Co-PI for "Reusable Hypersonic Vehicle Structures," sub-contract from The University of Dayton Research Institute, $893,239.
2. Principal Investigator for "Heterogeneous HPC for High-order Stabilized Finite-elements on Moving and Deforming Domains," funded by Engility Corporation; 01 September, 2017 – 31 August, 2019; $421,997.
3. Principal Investigator for "Computational Simulation of the Purdue 3-stage Experimental Core Compressor," funded by Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering; 01 July, 2015 – 30 June, 2016; $80,591.
4. Co-Investigator for "Validated Aerodynamic Analysis and Design Tools for Integrated Embedded Aircraft Propulsion Systems," funded by NASA Glenn Research Center; August, 2007 – August, 2010; $1,527,000.

Contact Information

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Chattanooga, TN 37403.
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Occupation: Assistant professor - (June 2016 to present**)** University of Tennessee, Chattanooga, Department of Mathematics

Education

Ph.D., Mathematical Sciences (Operations Research), December 2013, Clemson University, Clemson, SC.
M.Sc., Mathematical Sciences, August 2009, Clemson University, Clemson, SC.
B.Sc. (Hons), Mathematics, April 2003, University of Peradeniya, Sri-Lanka.

Teaching Experience

1. **Assistant professor*** - (June 2016 to present) University of Tennessee, Chattanooga, Department of Mathematics
2. **Assistant professor (Limited Term)** * - (August 2015 to May 2016) Department of Mathematics and Computer Science, Albany State University
3. **Lecturer*** - (August 2014 to May 2015) Department of Mathematics, Kennesaw State University
4. **Visiting Lecturer*** - (January 2014 - May 2014) Department of Mathematical Sciences, Clemson University

Research Experience

1. **Weerasena L***., Wiecek M.M., A Tolerance Function for the Multiobjective Set Covering Problem, submitted to *Optimization Letters* in February 2018
2. Bandara D., **Weerasena L***., Metaheuristic Algorithms to Solve the Reserve Design Problem, *International Conference on Enterprise Marketing and Globalization (EMG). Proceedings. Global Science and Technology Forum, (2016), 107:111*
3. Vanderpooten D*., **Weerasena L**., Wiecek M.M., Covers and approximations in multi-objective optimization, *Journal of Global Optimization, (2016), 1:19*
4. Soylu B., **Weerasena L***., Wiecek M.M., An algorithm for approximating the Pareto Set of the multiobjective set covering problem, *Annals of Operations Research, (2016), 1:22*
5. Shier D., Tonkyn D., **Weerasena L***., A Hierarchical approach to designing compact ecological reserve systems, *Environmental Modeling and Assessment, (2014), 19(5):437-449*

6. **Impact of Engineered Nanoparticles on the Growth of Roots**, (Palchoudhury S.*, Gharge U., Albattah A., Miller J., Ketan Patel K.,Patrick E., Santiago , Holler R., **Weeraena L**., and Jungjohann K.) intent to submit to *Nanoscale* in March 2018.
7. **Local search tolerance function for the multi-objective combinatorial optimization problems** (Lakmali Weerasena*), intent to submit to *Journal of the Operational Research Society* in March 2018.

**First author*

Invited Talks

1. **A cost to coverage ratio based heuristic algorithm for the multi-objective set covering problem,** *INFORMS Conference,* October 2017, Texas, USA
2. **Designing of spatially compact ecological reserve systems**, *Undergraduate Seminar, Department of Biology, Geology and Environmental Science*, October 2017, University of Tennessee at Chattanooga, Tennessee, USA
3. **Local branching algorithm for approximating the Pareto set of the multi-objective set covering problem**, *INFORMS Conference,* November 2016, Tennessee, USA

Presentations since 2015

1. **A Local-search Algorithm and a Tolerance Function for multi-objective combinatorial optimization problems**, *Math Colloquium, Department of Mathematics*, October 2017, University of Tennessee at Chattanooga, Tennessee, USA
2. **An approximation algorithm for the multi-objective combinatorial optimization problems**, *24th International Conference on Multiple Criteria Decision Making*, July 2017, Ottawa, Canada
3. **Approximation algorithm for the multi-objective set covering problem**, *Math Colloquium, Department of Mathematics*, November 2016, University of Tennessee at Chattanooga, Tennessee, USA
4. **Comparison of meta-heuristic algorithm performances**, *Graduate Research Symposium*, April 2016 Albany State University, Albany, GA, USA
5. **An approximating algorithm for the multi-objective set covering problem**, *AMS/Sectional meeting,* March 2016, Atlanta, Georgia, USA

Grants and Awards

1. Faculty Grant, University of Tennessee at Chattanooga, 2016, 2017
2. Travel Grant, Department of Mathematics, University of Tennessee at Chattanooga, 2016, 2017
3. Undergraduate Research Grant (Student, Nichols Graham), Albany State University, 2016
4. Professional Enrichment Grant, Clemson University, 2011, 2012
5. Commendable presentation, Peradeniya University Annual Research Session, 2005

Weidong Wu, PhD: Project PI
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(a) PROFESSIONAL PREPARATION

- Huazhong University of Science & Technology Civil Engineering B.S., 1994-1998
- University of Mississippi Civil Engineering Ph.D., 2003-2008
- University of Mississippi Computer Science Master Core Courses 2009-2012

(b) APPOINTMENTS

- 2013-Present, Assistant Professor / Civil Engineering**,** University of Tennessee at Chattanooga.
- 2013, Senior FEA Engineer, Comau Inc (A FIAT company)
- 2008-2012, Postdoc / Civil Engineering, University of Mississippi.
- 1999-2003, Structural Engineer, Wuhan Linyun Sci & Tech. Co. Ltd. China

(c) PUBLICATIONS

publications

1) Wu, W., Qurishee, M. A., Owino, J. O., Fomunung, I. W., Onyango, M. A. (2018) "Deep learning based concrete bridge deck and pavement damage identification using unmanned aerial vehicle" (pending journal paper)
2) Wu, W., Owino, J. O., Fomunung, I. W., Onyango, M. A. (2018)" Multilevel Micromechanics Modeling of Modeled Recycled Aggregate Concrete" *ASCE Engineering Mechanics Institute Conference 2018, May 29-June 1 MIT* (pending conference).
3) Qurishee, M. A., Wu, W., Owino, J. O.,(2018) "Non-Destructive Test Application in Civil Infrastructure: A Review" Co-authored with graduate student Murad Qurishee.(pending journal paper)
4) W Onyango, M. A., Merabti, S. A., Owino, J. O., Fomunung, I. W., Wu, W. (2017). Analysis of cost effective pavement treatment and budget optimization for arterial roads in the city of Chattanooga. *Frontiers of Structural and Civil Engineering*, 1--9.
5) Liang,Y. , Wu, D., Liu, G., Li.,Y., Gao, C.,Ma,Z., **Wu,W**., (2016), "Big data-enabled multiscale serviceability analysis for aging bridges", *Digital Communications and Networks*, *2*(3), 97-107.

Other significant publications

1) Wu, W., Al-Ostaz, A., Gladden, J., Cheng, A. H.-D., and Li, G. (2010), "Measurement of mechanical properties of hydrated cement paste using resonant ultrasound spectroscopy," *Journal of ASTM International*, 7(5)
2) Al-Ostaz, A., Wu, W., Alkhateb, H. and Alzebdeh, K.I. (2009), "Joint effect of shape and size on progressive damage of random composites," *Computational Material Science*, 46(4), pp. 1141-1151.
3) Al-Ostaz, A., Wu, W., Cheng, A. H.-D. and Song, C.R. (2009), "A molecular dynamics and microporomechanics study on the mechanical properties of major constituents of hydrated cement," *Composites B*, 41(7), pp. 543-549.
4) Wu, W., Al-Ostaz, A., Cheng, A. H.-D. and Song, C.R. (2010), "Concrete as a hierarchical structural composite material," *International Journal for Multiscale Computational Engineering*, 8(6), pp. 585-595.
5) Wu, W., Al-Ostaz, A., Cheng, A. H.-D. and Song, C.R. (2011), "A molecular dynamics study on the mechanical properties of major constituents of Portland cement," *ASCE Journal of Nanomechanics and Micromechanics*, 1(2), pp 84-90.

(d) SYNERGISTIC ACTIVITIES

1) Serving editorial board of *Civil Engineering Journal*
2) Serving as book reviewer for *CRC Press*
3) Reviewer, *Journal of Cleaner Production*.
4) Committee Member, National Institute of Technology, Warangal, Warangal, Telangana.
5) Member of *American Society of Civil Engineer*
6) Served as conference track chair, 1st International Conference on Theoretical, Analytical and Computational Methods for Composite Materials and Composite Structures (2017)
7) Developed an online based course

(e) CONTRACTS, GRANTS AND SPONSORED RESEARCH

- TBAEE Laboratory Equipment Grant for Civil Engineering, Sponsored by Tennessee Board of Architectural and Engineering Examiners, State, $28,863.32. (PI).
- Traffic data input for mechanistic empirical pavement design guide for Tennessee, Sponsored by TDOT, State, $172,053.80. (Co-PI).
- Computer modeling of PolyLEVEL for highway pavement leveling, Sponsored by Ruth S. Holmberg Grants for Faculty Excellence, The University of Tennessee at Chattanooga, $5,000.00. (PI).

Mengjun Xie's Biographical Sketch

A. Professional Preparation

- East China Normal University Shanghai, China B.Eng. in Computer Science 1999
- East China Normal University Shanghai, China M.Eng. in Computer Science 2002
- College of William and Mary Virginia, USA Ph.D. in Computer Science 2010

B. Appointments

- July 2016–Present Associate Professor of Computer Science
  University of Arkansas at Little Rock, Little Rock, AR
- Aug. 2010–June 2016 Assistant Professor of Computer Science
  University of Arkansas at Little Rock, Little Rock, AR

C. Products

i. Products Most Relevant to this Proposal:

1. Yanyan Li and **Mengjun Xie**, "Understanding Secure and Usable Gestures for Realtime Motion based Authentication," in *Proceedings of the IEEE INFOCOM 2018 Workshops, The 2nd IEEE International Workshop on the Security, Privacy, and Digital Forensics of Mobile Systems and Networks (MobiSec'18)*, pp. 13–20, 2018.
2. Yanyan Li, **Mengjun Xie**, and Jiang Bian, "SegAuth: A Segment-based Approach to Behavioral Biometric Authentication," in *Proceedings of 2016 IEEE Conference on Communications and Network Security (CNS'16)* , pp. 15–23, 2016.
3. Junshuang Yang, Yanyan Li, and **Mengjun Xie**, "MotionAuth: Motion-based Authentication for Wrist Worn Smart Devices," in *Proceedings of the Workshop on Sensing Systems and Applications Using Wrist Worn Smart Devices*, pp. 50–55, 2015.
4. **Mengjun Xie**, Yanyan Li, Kenji Yoshigoe, Remzi Seker, and Jiang Bian, "CamAuth: Securing Web Authentication with Camera," in *Proceedings of the 16th IEEE International Symposium on High Assurance Systems Engineering*, pp. 232–239, 2015.
5. **Mengjun Xie**, Zhenyu Wu, and Haining Wang, "Secure Instant Messaging in Enterprise-like Networks," in *Computer Networks*, volume 56, issue 1, pp. 448–461, 2012.

ii. Other Significant Publications:

1. Yanyan Li, Dung Nguyen, and **Mengjun Xie**, "EZSetup: A Novel Tool for Cybersecurity Practices Utilizing Cloud Resources," in *Proceedings of 18th ACM Annual Conference on IT Education (SIGITE'17)*, pp. 53–58, 2017.

2. Yanyan Li and **Mengjun Xie**, "Platoon: A Virtual Platform for Team-oriented Cybersecurity Training and Exercises," in *Proceedings of 17th ACM Annual Conference on IT Education (SIGITE'16)*, pp. 20–25, 2016.
   The Platoon platform has been released as an open-source project and it can be freely accessed at `https://www.mengjunxie.org/cyberdefense/`. The platform has been shared with 20 education institutions and professionals in 7 countries.

3. Yue Zhao, Kenji Yoshigoe, Jiang Bian, **Mengjun Xie**, Zhe Xue, and Yong Feng, "A Distributed Graph-Parallel Computing System with Lightweight Communication Overhead," in *IEEE Transactions on Big Data*, vol. 2, issue 3, pp. 204–218, 2016.
4. Jiang Bian, **Mengjun Xie**, Teresa J. Hudson, Hari Eswaran, Mathias Brochhausen, Josh Hanna, and William R. Hogan, "CollaborationViz: Interactive visual exploration of biomedical research collaboration networks," in *PLoS ONE*, vol. 9, issue 11, e111928, 2014.
5. Zhenyu Wu, **Mengjun Xie**, and Haining Wang, "On Energy Security of Server Systems," in *IEEE Transactions on Dependable and Secure Computing (TDSC)*, vol. 9, issue 6, pp. 865-876, 2012.

D. Synergistic Activities

The highlights of PI's experiences and leadership in security research and education include:

1. **He has published over 30 peer-reviewed papers on cybersecurity in major security and systems conferences and journals** including ACM CCS, USENIX Security, USENIX NSDI, IEEE INFOCOM, IEEE CNS, SecureComm, IEEE/ACM Transactions on Networking, IEEE Transactions on Dependable and Secure Computing, etc. **His research has been funded by NSF and NSA.** He received Faculty Excellence Award in Research and Creative Endeavors from College of Engineering and Information Technology (EIT) at UA Little Rock in 2017.
2. He has served on Technical Program Committee for numerous international security and system conferences and he also has served as editor/reviewer for various international journals on security and networking. He co-organized the 8th Central Area Networking and Security (CANSEC) Workshop and the affiliated Cyber Defense Competition in 2015 and the 1st Workshop on Mobile Cloud Computing in Healthcare in 2013. The Cyber Defense Competition attracted 38 undergraduate and graduate students from 7 universities in Missouri, Kansas, Tennessee, and Arkansas.
3. **He serves as the Director of DHS/NSA designated Center of Academic Excellence in Cyber Defense and the Director of Computational Research Center at UA Little Rock. He also serves on UA Little Rock System Incident Response Team as the only faculty representative.** He also founded and directs the Cyber Security Club at UA Little Rock. Under his guidance, UA Little Rock won 3rd place in 2016 Southwest Collegiate Cyber Defense Competition (CCDC).
4. **He has extensive and outstanding mentoring and advising experiences at all levels: high school, undergraduate, and graduate levels.** He has mentored 5 high school students on mobile computing in 2013-2017 summers through the High School Research Program of EIT College and 8 undergraduates from other universities in 2014-2016 summers through NSF REU program. He also advised two African American students in the past. The internal student through EIT summer research program was awarded prestigious NSF Graduate Fellowship and the external student through NSF REU program received the Best Poster Award from IEEE CNS 2016. Two of his Master's students received college-level Outstanding MS Student Award and and his PhD student, Yanyan Li, received Outstanding PhD Student Award multiple times.

Appendix B

Awardee Project Reports

New Projects for FY 2019

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Lead PI: Dr. Vahid Disfani

Co-PI(s): Dr. Mo Ahmadi, Dr. Mina Sartipi

Project Title: Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design

Date Submitted: 03/05/2018

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

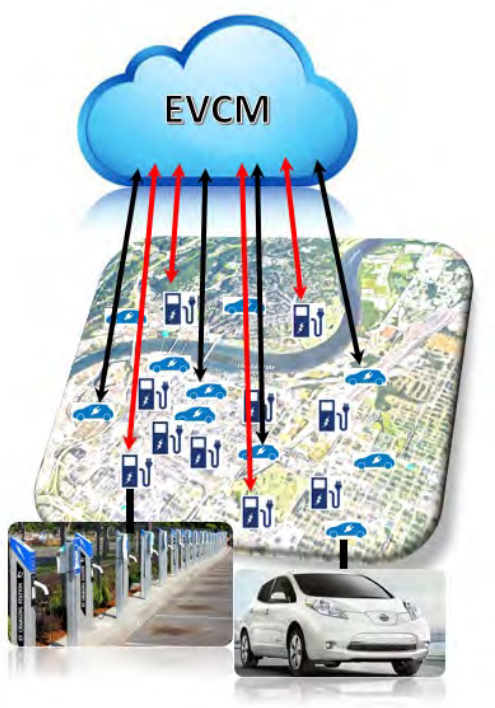
Growing interest in electric vehicles (EV) has established an inevitable demand for installation and smart operation of electric vehicle supply equipment (EVSE), also known as charging stations. Maximizing utilization of EVSEs is a sustained challenge in EVSE operations despite the emergence of EV station locators, e.g. PlugShare.com and ChargeHub.com, providing EVSEs' availability and price information which are partial, real-time, and snapshot datasets. More significantly, the missing key element in this platform is the lack of communication from demand side or EVs. These challenges often leave EVs—sometimes desperate for charging—disconnected while several EVSEs are available nearby.

Although the corresponding literature includes a significant number of works in the optimal charging process and schedule of EVs and their technical and economic effects on power system and electricity markets, none of them has studied how to match the EVs and EVSEs to maximize the social welfare of both parties. These social benefits will at least include higher utilization of EVSEs as well as time savings and less costs for EV owners. The fact that the literature is silent on this issue and that the EVs are becoming the main core of the near future road transportation platform make this period of time a critical and favorable moment to investigate reliable solutions to optimally match EVs and EVSEs for charging process.

PROJECT TITLE

Technology Area of Interest: Grid Integration of Electric Vehicles

PROPOSED TECHNICAL APPROACH	OUTCOMES
This project aims to computationally model and design EV charging markets (EVCM), which simultaneously gather demand data including desired destinations, bidding data, connection period, and energy demand and supply or EVSE availability and bidding data to optimally match supply and demand to maximize social welfare. • Task 1- Develop EV and EVSE growth models • Task 2- Design EV charging market (EVCM): Analytical Approach • Task 3- Simulate EVCM on software platforms and analyze short-term and long-term benefits	1 research presentations: Vahid Disfani, “Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design” in 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019. 4 posters: 1. Sakineh Khalili, Timothy Barczak, Chanda Kelly, Vahid Disfani, Mo Ahmadi, “Growth Modeling of Electric Vehicle Charging Demand in Chattanooga - A Case Study,” in 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019. 2. Sakineh Khalili, Timothy Barczak, Chanda Kelly, Vahid Disfani, Mo Ahmadi, “Growth Modeling of Electric Vehicle Charging Demand in Chattanooga - A Case Study,” in 2019 UTC CECS Technology Symposium, Chattanooga, TN, April 2019. 3. Saroj Khanal, Sakineh Khalili, Farog Mohamed, Shailesh Wasti, Vahid Disfani, Mo Ahmadi, Mina Sartipi, “Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design” in 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019. 4. Saroj Khanal, Sakineh Khalili, Farog Mohamed, Shailesh Wasti, Vahid Disfani, Mo Ahmadi, Mina Sartipi, “Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design” in 2019 UTC CECS Technology Symposium, Chattanooga, TN, April 2019.

RESULTS	OTHER INFO
	**Budget and Schedule** Total Budget: $ 96,114.00 Actual Used: $ 92,347.19 Balance: $ 3,766.81 Total period of performance is 12 months. Task 1: Months 1-4 Task 2: Months 4-8 Task 3: Months 7-12 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 • Internal poster presentations **Organization Information** *615 McCallie Ave., Dept 2342* *University of Tennessee at Chattanooga* *423-425-4354* *Vahid-disfani@utc.edu*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop EV and EVSE growth models	We collected data of EVSEs in Chattanooga, including location, size, and operators. We also collected historical data of EV charging events in the city of Chattanooga from CARTA. We developed spatio-temporal growth models for EV charging demand for the city using current EV demand and population density
Design EV charging market (EVCM): Analytical Approach	We determined necessary parameters affecting EVs and EVSEs bidding process, such as connection time, energy demand, and proximity to destination, to identify objective functions and different constraints of both EVs and EVSEs for market clearing process. The objective functions are selected as maximizing utilization of EVSEs, maximizing social welfare of demand side, and minimizing walking distance. The constraints are

	identified as deliverability of energy demand, maximum walking distance, and demand budget. We used MATLAB to model and solve the optimization problem with multiple EVSE and multiple EV demands. The optimization problem is modeled efficiently to be solved for variable number of EV demands, number of EVSEs, horizons, and time intervals in reasonable times.
Simulate EVCM on software platforms and analyze short-term and long-term benefits	We developed time-domain (real-time) simulation platforms in MATLAB to model stochastic properties of EVs' demand and EVSEs' availability using data collected in Task 1. We developed Monte-Carlo simulation platforms in MATLAB to study the long-term impact of the market designed. Multiple simulations with variable time interval, number of EV demands, and market intervals are performed to (1) analyze EVCM efficiency and its short-terms impacts using time-domain platforms, and (2) to quantify long-term benefits of EVCM in reduction of energy consumption and environmental emissions.

Challenges & Strategies Used to Address / Overcome:

As anticipated in the proposal, the main challenge was access to some data that we deemed available at the time we wrote the proposal. Some data were not readily available when we tried to collect. The dataset of EV charging events for the last 3 years was a great set of data that we could get access through CARTA. CARTA shared data of the 63 EVSEs that it owns in Chattanooga and we could use it for our research very 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 were expecting—even at the current level of EV charging demand—to see higher long-term impacts if people start to use the designed market instead of finding charging stations by searching. However, the simulation results show that the fuel cost and emission reductions in just one year can easily cover the implementation costs of the designed market.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

Dr. Vahid Disfani (PI): This research grant funded through CEACSE helped the PI to make this topic of research one of the research trends in his research. One PhD student is joining Dr. Disfani's research group to continue this research. With the increasing interest in EVs and

academic/industrial research on EV, this grant is going to be even more fruitful for the PI's future research works.

Dr. Mo Ahmadi: He designed a course project for a group of students in his data analytics class. The students successfully managed the first task of this project. This research grant helped Drs. Ahmadi and Disfani build a good collaboration between their research groups in the College of Business and the College of Engineering and Computer Science for future research.

Dr. Sartipi: She was a good help in getting access to some data. This research topic might be one of the topics in her research team. Dr. Sartipi and the PI will continue to collaborate on this project.

Students Impacted

Saroj Khanal: Saroj was a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He was involved in all tasks of the project. He learned data processing and data visualization techniques. He learned development of optimization problem models and their solution using optimization solvers in MATLAB. He graduated in summer. The optimization knowledge he earned through this project enabled him to peruse his next career with the microgrid optimization group at National Renewable Energy Laboratory (NREL).

Shailesh Wasti**:** Shailesh is a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He was involved in all tasks of the project. He learned data processing and data visualization techniques. He learned development of optimization problem models and their solution using optimization solvers in MATLAB. He still has one year to graduate. His future research will be directly related to the topic of this project.

Farog Ahmed: Farog is a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He was involved in Tasks 2 and 3 of the project. He learned data processing and data visualization techniques. He learned development of optimization problem models and their solution using optimization solvers in MATLAB. He still has one year to graduate. His future research will most likely be different from the topic of this project.

Sakineh Khalili: Sakineh is an MBA student and research assistant for Dr. Ahmadi in the college of business. She was involved in Task 1 of the project. She learned data processing and data visualization techniques using Tableau. She learned how to perform statistical analysis on the EV demand empirical data to develop. The knowledge she obtained through this project enabled her to be hired as a business data analyst by the Covenant Transport, Inc. Sakineh still has one year left before she graduates.

Ahmad Eltayeb: Ahmed helped the project by developing time-domain simulation platforms in MATLAB Simulink. He learned how to apply optimization techniques in these platforms. His research enabled him to be hired by Mesa Associates, Inc. in Chattanooga.

Community and Broader Impacts

We have shown in this project that implementation of the market designed leads to potential societal benefits for the community. Once implemented, EVCM will enable people to find EV

charging stations for their demand well in advance with minimum anxiety. This helps EV owners spend less time on the road to find vacant EVSE for their charging demand. It also leads to less electrical energy consumed, less environmental emissions, and less energy costs.

One of the challenges of EV charging optimization and EV impact study on power grid is the uncertainty of the time and location of EV connection to the grid. EVCM and its popularity between EV owners are expected to reduce this uncertainty and enable the EVSE owners to optimize their charging process to maximize their benefits. EPB can also plan for the potential loads in advance (days/weeks/months ahead) and design an efficient pricing strategy to direct EVSEs' optimal charging profiles to benefit the system.

Scholarly Products

Software:

1. One software package has been developed by the team. The package includes data cleaning, optimization platform, Monte-Carlo simulation, and post analysis sections to run the entire tasks of the projects.

Presentations at UTC:

Vahid Disfani, "Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design" in 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019.

Sakineh Khalili, Timothy Barczak, Chanda Kelly, **Vahid Disfani**, **Mo Ahmadi**, "Growth Modeling of Electric Vehicle Charging Demand in Chattanooga - A Case Study," in 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019.

Sakineh Khalili, Timothy Barczak, Chanda Kelly, **Vahid Disfani**, **Mo Ahmadi**, "Growth Modeling of Electric Vehicle Charging Demand in Chattanooga - A Case Study," in 2019 UTC CECS Technology Symposium, Chattanooga, TN, April 2019.

Saroj Khanal, Sakineh Khalili, Farog Mohamed, Shailesh Wasti, **Vahid Disfani**, **Mo Ahmadi**, **Mina Sartipi**, "Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design" in 2019 UTC ReSEARCH Dialogues, Chattanooga, TN, April 2019.

Saroj Khanal, Sakineh Khalili, Farog Mohamed, Shailesh Wasti, **Vahid Disfani**, **Mo Ahmadi**, **Mina Sartipi**, "Urban Electric Vehicle Charging Markets: Computational Modeling and Optimal Design" in 2019 UTC CECS Technology Symposium, Chattanooga, TN, April 2019.

Inventions or Other Intellectual Property

We have developed a software package throughout the project. The package includes data cleaning, optimization platform, Monte-Carlo simulation, and post analysis sections to run the entire tasks of the projects. The software product and methods developed through this project are novel and patentable. No invention disclosure or patent or copyright applications have been filed, but I consider to file one with SimCenter help. The timeline is not clear yet.

Research Outreach & Collaboration

Through this project, we created some collaborations between UTC, EPB and CARTA. These collaborations are expected to increase in the next rounds of this research. As soon as the market designed is publicly available and used by EV owners, research projects on EV charging optimizations and grid impact study will start. To implement the market in Chattanooga, the team is going to collaborate with ChargePoint as the biggest EVSE company in the US as well.

EXTERNAL FUNDING

Proposal Submissions

1. No proposal has been submitted yet.

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. I attended on-campus workshops on NSF CAREER proposal as well as several meetings with ORSP and SimCenter personnel to discuss potential proposals and future research activities.

WHAT'S NEXT FOR THIS RESEARCH?

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

This CEACSE will be followed by the following activities:

One year: I will submit an extramural proposal which leads to implementation of the market developed in this project. My research team will continue their research toward the follow-on research projects.

2 years: The plan is to work toward implementation of the market through the funded external grant. The follow-on research done in year 1 will be submitted to attract more extramural funds.

In 5 years, I expect to have the entire market implemented and publicly used by EV owners. By then, implementation of EVCM in Chattanooga can be a proof of concept for its implementation in other areas, especially more populated cities.

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

This grant will be followed up by some research projects. I expect to expand UTC's collaboration with EPB and CARTA toward implementation of this market in Chattanooga. To do so, I will collaborate with ChargePoint as well in order to apply required modifications on EVSEs. My research team will continue to study the impacts of the designed market on EPB power grid and on EV charging optimization process. We will also do research on fleet charging optimization for CARTA.

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

There were some remaining funds (4%) at the end of the project period. The reason was mainly due to the fact that my students could not work at times for various reasons such as internship and graduation, and I could not replace all my students with someone who could effectively help us the project.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Ignatius Fomunung, Lead PI

Co-PI(s): Arash Ghasemi, Joseph Owino, Mbakisya Onyango
Other Personnel: Babatunde Atolagbe, Graduate Student

Project Title: 3D Drone Delivery Transportation Problem

Date Submitted: 03/05/2018

Award Start – End Date: July 1, 2018 - June 30, 2019

Non-Technical Summary:

We have developed infrastructure theory and software required for urban modeling. These include codes for automatically generating surface mesh for a given urban system that accurately models the buildings using an unstructured watertight surface mesh. We have also investigated routing and energy reduction strategies.

The primary purpose of these codes was to be used in determination of drone routing; however, the results can be applied to a wide range of problems in the area of urban modeling, including evacuation planning, hazardous plume and inverse problems, routing for minimizing fuel efficiency, etc. Currently, the team has developed two internal presentations, one presentation in China, and an article that has been submitted to the Transportation Research Board annual conference for presentation and publication. One graduate student was supported during this research, and he has completed his master's thesis in this field.

3D Drone Delivery Transportation Problem

Technology Area of Interest: drone delivery, transportation, energy efficient

PROPOSED TECHNICAL APPROACH	OUTCOMES
• The cityscape can be modeled automatically using special algorithms—no need to use CAD software and model manually. • For the drone delivery problem, the existence of buildings and obstacles in an urban area generates regions of wakes that could yield aerodynamic advantage to save energy.	A series of algorithms and software are developed that help us to automatically model an urban landscape. Techniques to take advantage of the wake regions to save energy are presented. Two internal presentations, two external presentations, and one article have been produced. The second external presentation will take place in October in Dubai, UAE, at the Applied Science and Technology Conference as invited speaker.
RESULTS	**OTHER INFO**
Techniques to take advantage of the wake regions to save energy are presented. One internal presentation, one external presentation, and one article have been developed.	**Budget and Schedule** Total Budget: $67,568.00 Actual Used: $61,795.47 Balance: $5,772.53 Total period of performance is 12 months. Literature Review: Months 1-6 Developing OSM reader: Months 3-6 Developing automatic mesher: Months 6-12 Routing and documentation: Months 8-12 **Deliverables** • Monthly reports • Currently delivered three presentations and an article. Team is currently working on integration and validating the results, which will be used for another article, and preparing an external grant proposal. • B. Atolagbe, A. Ghasemi, I. Fomunung, M. Onyango and J. Owino, “Towards Energy-Optimized Deployment of Unmanned Aerial Vehicles for Civil Applications: A Novel Conceptual Framework”, Submitted to Transportation Research Board on Submission Date: July 31st, 2019 • External and internal conference presentation: 1- Research Dialogues 2019; 2- the 2019 CECS technology symposium; 3- presentation at the 19th

	COTA International Conference of Transportation Professionals in Nanjing, China, July 2019; 4- Presentation at the 3rd Global Conference and Expo on Applied Science, Engineering and Technology applied science and technology conference in October 2019, Dubai, UAE. Title of talk: Energy-Optimized Routing with Application in Delivery Drones.

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Arbitrary building footprints in any geographic location can be obtained by using the OSM database, which is publicly and freely available.	A code is developed in C from scratch to query OSM databases and obtain building footprints inside and arbitrary bounding box specified by GPS coordinates
Arbitrary height and topography elevation information can be obtained and rearranged automatically from LIDAR data	A C code is developed to achieve this purpose
The footprints can be extruded according to the building heights specified in the database	A series of algorithms and MATLAB codes are developed to successfully achieved this purpose
Topography elevation and building footprints can be merged together to obtain an accurate and realistic surface representation of the urban landscape	We developed a mathematical relation that merges these data together. A series of algorithms and MATLAB codes are developed to successfully achieve this purpose.
Volumetric tetrahedral mesh can be generated automatically using the surface mesh without needing to use a commercial software.	We used/developed a series of codes that achieve this goal. This resulted in an in-house tool-chain to solve a range of problems like this.

Challenges & Strategies Used to Address / Overcome:

It was originally planned to model the details of ceilings/roofs of the buildings.

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

While the OSM database just recently introduced a standard to represent the details of the roofs, these data and the corresponding standard is in experimental/pilot stage. The team decided to model the buildings without including these details.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The PI and Co-PIs are actively working on this framework to further incorporate it in the departmental research and activities both at the graduate and undergraduate levels.

Students Impacted

Mr. Babatunde Atolagbe, the graduate student on this project, has gained a high-level knowledge of programming, software development, geometric modeling, and documentation skills. The grid generation code developed in this project has a significant work load that is usually defined as a separate master's thesis in the field of computational engineering and computer science. He successfully mastered how to implement all algorithms and integrate them into some applications in the field of civil engineering. He also used the codes to generate a grid for a part of the Tennessee River used in Dr. Bathi's research.

Community and Broader Impacts

None.

Scholarly Products

Developed Software:

1. Building Footprint Capture: A C89 code to obtain the building footprints inside a bounding box specified by GPS coordinates.
2. LiDAR converter: A C89 code to process USGS topography data.
3. Auto City Generator: A set of MATLAB functions to create watertight unstructured surface mesh for an urban landscape.

External Conferences:

B. Atolagbe, **A**. **Ghasemi**, **I**. **Fomunung**, **M**. **Onyango** and **J. Owino**, "Towards Energy-Optimized Deployment of Unmanned Aerial Vehicles for Civil Applications: A Novel Conceptual Framework," Submitted to Transportation Research Board on Submission Date: July 31st, 2019

Presentations at UTC:

B. Atolagbe, A. Ghasemi, I. Fomunung, M. Onyango and J. Owino, "Three-dimensional mesh representation of urban environment based on OpenStreetMap (OSM) data," 2019 ReSEARCH dialogue, University of Tennessee and Chattanooga.

Atolagbe, A. Ghasemi, I. Fomunung, M. Onyango and J. Owino, "City Modeling based on actual OSM data," 2019 Technology Symposium, Chattanooga TN.

Inventions or Other Intellectual Property

Not Applicable.

Research Outreach & Collaboration

Generating grids for a part of the Tennessee River used in Dr. Bathi's research group: We used our code to generate a suitable grid that can be used as an input file for TVA software. This enables them to accurately analyze the flow field in the part of river they are currently investigating.

EXTERNAL FUNDING

Proposal Submissions

None

Contracts/Awards Received

None

Sponsored Program Capacity Building Activities

1. Attended a meeting with a TVA sponsor organized by Mr. Bonfiglio. Possibility of mutual collaboration was discussed.
2. The PI attended a NIH workshop, "Writing Winning NIH Grant Proposals" on September 12, 2018 on UTC campus.

WHAT'S NEXT FOR THIS RESEARCH?

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

Work continues on the project even though the grant period has expired. The objective is to obtain some robust preliminary results, which will be used to write a proposal to an external funding agency.

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

1. Automatically modeling river geometry and bottom topography using our currently developed codes. This could be a potential research collaboration with Dr. Jejal Bathi, UTC Chemical Engineering, and Dr. Sreenivas, UTC Mechanical Engineering.

2. The code developed as part of this project could be adapted and applied to the deployment of charging stations to support expansion of use of electric vehicles. This is a needed and promising area of research, which we will pursue.

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

The ultimate solution to the problem of optimizing route choice for drones by considering energy efficiency is being evolved through the use of concepts from across many engineering disciplines, from civil engineering to computer science to computational fluid dynamics and simulation, thus presenting an opportunity to build a truly multidisciplinary collaboration team.

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

Currently, we cannot determine them.

FINANCIAL ACCOUNTING

The remaining funds, $5,773.52 were mainly budgeted for benefits. It seems there is some difficulty in precisely figuring out how much exactly is needed for benefits.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Lead PI: Sumith Gunasekera, Ph.D., Associate Professor of Statistics

Co-PI(s): Lakmali Weerasena, Ph.D. Hong Qin, Ph.D.

Other Personnel: Aruna Saram, MS, MBA, Doctoral Candidate in Computational Science with concentration in Computational & Applied Mathematics

Project Title: Estimating the Youden Index Under the Multivariate Roc Curve in The Presence of Missing Values of Mass Diseased And Healthy Biomarker Data

Date Submitted: 02/27/2018

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

Multivariate Youden index (J) and its corresponding optimal cut-point (c^*) have become the most effective and efficient approach in multi-biomarker mass data analysis to distinguish diseased from the healthy in this digitized era. However, the existing statistical classical approach does not produce exact solutions in the presence of nuisance parameters and missing and group mass data. This proposed novel high-performing computational-based generalized Variable Method is an alternative procedure to produce exact statistical inferential results for J and c^* in the presence of such constraints.

In compliance with the mission of the Center of Excellence in Applied Computational Science and Engineering (CEACSE) at The University of Tennessee at Chattanooga (UTC) that is to establish and expand a cohesive multidisciplinary effort in applied computational science and engineering leveraging across UTC and produce sustained growth in research funding, excellence in integrated education and research, and to increase national and international stature and competitiveness in Tennessee, we built a high-performance computational re-source as part of a web services framework called GeneralizedMultivariateYouden (GMY) that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers in the presence of missing and grouped, or pooled, data. Codes of GMY were written in Python for the multivariate-BioMarker (mBM) data.

PROJECT TITLE: ESTIMATING THE YOUDEN INDEX UNDER THE MULTIVARIATE ROC CURVE IN THE PRESENCE OF MISSING VALUES OF MASS DISEASED AND HEALTHY BIOMARKER DATA

Technology Area of Interest: Big Data, Networking, Artificial Intelligence (AI), Machine Learning, (ML), Deep Learning (DL)

PROPOSED TECHNICAL APPROACH	OUTCOMES
Summary statement: Multivariate Youden index (J) and its corresponding optimal cut-point (c^*) have become the most effective and efficient approach in multi-biomarker mass data analysis to distinguish diseased from the healthy in this digitized era. However, the existing statistical classical approach does not produce exact solutions in the presence of nuisance parameters and missing and group mass data. This proposed novel high-performing computational-based generalized Variable Method is an alternative procedure to produce exact statistical inferential results for J and c^* in the presence of such constraints. List of tasks: • Analyze the Mammographic data and build theoretical aspects to improve the statistical procedure to enhance the efficiency of the Malignant (or Breast Cancer) patients' classification • Intensive and extensive data analyses and simulation studies will be performed for hypothesis testing and the interval estimation of the multivariate Youden index (J) • Different aspects of this research would utilize as Doctoral Dissertations, Master's Theses, Undergraduate Honors Theses, and/or REU (Research Experience for Undergraduate) Projects • Several manuscripts based on the results of this project will be submitted to top peer-reviewed (refereed) statistical or biomedical journals, such as *Statistics in Medicine,*	• Publishing one (1) Paper • Preparing two (2) or more Manuscripts • Conference Participation 1. Invited Keynote Speaker at the 8th International Conference on Biostatistics & Bioinformatics (CB&B) from September 16–17, 2019 in San Francisco, CA, USA. 2. Invited Speaker at the 7th International Conference on Biostatistics & Bioinformatics (CB&B) held September 26–27, 2018 at Holiday Inn Chicago O Hare, Chicago, Illinois, USA. 3. Invited Speaker at the Joint Statistical Meetings (JSM) from July 27–August 01, 2019 in Denver, Colorado, USA. • Scholarly and Pedagogical works at the Research Dialogues 2019 at UTC • Preparation of: 1. One (1) internal grant in CEACSE 2020/21 2. Three (3) External Grants in NSF-REU, NSF-RUI, NIH-R15-AREA or REAP 3. Podium Talk, Panel Talk, Elevator Pitch Talk, Poster: Research Dialogues 2020

Computational Statistics & Data Analysis, and Biometrics • Papers stemming from this research will be presented at the 2019 Joint Statistical Meetings (JSM)	
RESULTS	**OTHER INFO**
Building modular high-performance computational resources as part of a web services framework called GeneralizedMultivariateYouden (GMY) that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers in the presence of missing and grouped, or pooled, data. Codes were written in Python are supported by a relational database such as MySQL.	**Budget and Schedule** Total Budget: $97,901.00 Actual Used: $95,416.16 Balance: $ 2,484.84 Total period of performance is 12 months. Task 1, 2: Months 1-6 Task 2: Months 6-12 Task 3, 4: Months 6-12 Task 5: 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

ACCOMPLISHMENTS & OUTCOMES

Project Overview:

The common problem of interest in classification is allocating an individual or object to one of the predefined groups (or populations) by using a threshold. These problems were addressed by using a performance tool, namely a Receiver Operating Characteristic (ROC) Curve. Its expansion to other fields was prompt. The Youden index is a frequently used summary measure of the ROC curve. It both measures the effectiveness of a diagnostic marker and enables the selection of an optimal threshold value (cutoff point) for the biomarkers. The proposed research demonstrates how the Youden index for the 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 the breast cancer and by intensive and extensive computations of the simulated mass data with the aid of generalized variable method due to Tsui and Weerahandi (1989) (see also Weerahandi (1995, 2004), Gunasekera (2018, 2017, 2016, 2015) and Gunasekera and Ananda (2015)). 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 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 and the associated optimal cut-off point for the multi-biomarkers with missing data, where missing data are cleaned or tackled with the aid of imputation. These are juxtaposed using confidence intervals, p-values, power of the test, size of the test, coverage probability, bias, and root mean square error with a wide-ranging simulation study featuring a selection of various scenarios and the real-world breast cancer data.

List of Objective/Aims/Major Milestones Proposed:

We take this moment to thank Prof. Joanne Romagni, The Vice Chancellor for Research and Dean of the Graduate School, Prof. Anthony Skjellum, Professor and Director, SimCenter (Center of Excellence for Applied Computational Science and Engineering (CEACSE)), Prof. Michael Colvin, Former Interim, Head, Department of Mathematics, Ms. Anna Lane, Accounting Coordinator for the Vice Chancellor of Research & Dean of the Graduate School, and Ms. Heather Heinlein, Administrative Specialist, Department of Mathematics at UTC for their unstinted effort to support and strengthen our careers at UTC by providing this CEACSE 2018/19 Grant that resulted in:

- Building modular high-performance computational resources as part of a web services framework called GeneralizedMultivariateYouden (GMY) that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers in the presence of missing and grouped, or pooled, data. GMY provides efficient data uploading and access and a suite of high computations on multivariate Youden index and its corresponding optimal cut-point, and Receiver Operating Characteristic (ROC) curve analysis code that can be used or adapted for any species, individuals, entities, or any electrical, electronic, or mechanical components. Code was written in Python and is supported by a relational database such as MySQL (Structured Query Language (SQL) named after one of the co-founder's daughter MY, an open-source rational database management system (RDBMS)) that incorporates the largest coherent collection of multivariate-BioMarker (mBM) data.
- Publishing one (1) Paper:
    1. Gunasekera, S., Weerasena, L., Saram, A., Oluwakorede, A. (2019). Exact inference for the Youden index to discriminate individuals using two-parameter exponentially distributed pooled samples. *Biostatistics & Epidemiology* 3(1), 38–61, doi: 10.1080/24709360.2019.1587264
- Preparing two more Manuscripts:
    1. Gunasekera, S., Weerasena, L., Saram, A. (2019). Exact Inference for the Multivariate Youden Index to Discriminate Individuals using Normally Distributed Samples.
    2. Gunasekera, S., Weerasena, L., Saram, A. (2019). Exact Confidence Intervals for the Univariate Youden Index and Its Corresponding Optimal Cut-Point using Normally-, Mixture of Normally-, and t-Distributed Pooled Samples.
- Conference Participation:
    1. Invited Keynote Speaker at the 8th International Conference on Biostatistics & Bioinformatics (CB&B) sponsored by the Conference Series under the Theme *Exploring Advances in Biostatistics & Bioinformatics* from September 16–17, 2019 in San Francisco, CA, USA.

Gunasekera, S. (2019). Estimating the Youden index under the multivariate ROC curve in the presence of missing values of mass diseased- and healthy-biomarker data.

2. Invited Speaker at the 7th International Conference on Biostatistics & Bioinformatics (CB&B) sponsored by the Conference Series under the Theme *Exploring Advances in Biostatistics & Bioinformatics* held September 26–27, 2018 at Holiday Inn Chicago O 'Hare, Chicago, Illinois, USA.
Gunasekera, S. (2018). Exact inference for the Youden index to discriminate individuals using two-parameter exponentially distributed pooled samples.
3. Invited Speaker at the Joint Statistical Meetings (JSM) sponsored jointly by the American Statistical Association (ASA), International Biometric Society (IBS) (Eastern North American Region-ENAR and Western North American Region WNAR), Institute of Mathematical Statistics (IMS), Statistical Society of Canada (SSC), International Chinese Statistical Association (ICSA), International Indian Statistical Association (IISA), International Society for Bayesian Analysis (ISBA), Korean International Statistical Association (KISA), and Royal Statistical Society (RSS) under the Theme {\it Statistics: Making an Impact} from July 27–August 01, 2019 in Denver, Colorado, USA.
    (i) Gunasekera, S. (2019). Bayesian inference for the common-location parameter of several shifted-exponential populations.
    (ii) Wijekularathna, D. and Gunasekera, S. (2019). On Performing Generalized Inferences for the Burr XII Reliability Function based on Progressively Censored Data.

- Scholarly and Pedagogical works at the Research Dialogues 2019 at UTC:
    1. Poster Presentation: Gunasekera, S., Weerasena, L., Saram, A. Ajomobi (2019). Statistical Exploration of Stochastic Differential Equation Models used in the Stochastic Dynamics of Biological Systems: Statistical Algorithms & Computer Programs.
    2. Podium Talk: Gunasekera, S. (2018). Exact inference for the Youden index to discriminate individuals using two-parameter exponentially distributed pooled samples.
    3. Faculty Elevator Pitch: Gunasekera, S. (2019). Mathematics and Statistics: Who is the Winner?
- Preparation of:
    1. One (1) internal grant in CEACSE 2020/21.
    2. Four (4) External Grants in NSF-REU (Research Experience for Undergraduates) sponsored by the National Science Foundation (NSF), NSF-RUI (Research in Undergraduate Institutes) sponsored by the National Science Foundation (NSF), and NIH-R15-AREA (Academic Research Enhancement Award) or REAP (Research Enhancement Award) Programs sponsored by the National Institutes of Health (NIH), NIH/NSF-NIGMS/DMS grant opportunity by the National Institute of General Medical Science (NIGMS) of the National Institutes of Health (NIH) in collaboration with the Directorate of Mathematical Sciences (DMS) of the Division of Mathematical & Physical Sciences in the National Science Foundation (NSF) in collaboration with the UTC Faculty and Faculty from Troy University at Troy, Alabama, USA.
    3. Podium Talk, Panel Talk, Elevator Pitch Talk, Poster: Research Dialogues 2020
- Invitation of:
    1. Prof. Karunarthna Kulasekera, Assistant Dean for Academic Affairs, School of Public Health and Information System, and Professor & Chair of the Department of Bioinformatics and Biostatistics at the University of Louisville, Louisville,

Kentucky, USA, and former graduate coordinator in the Department of Mathematics & Statistics (presently School of Mathematical & Statistical Science) at Clemson University, for a research presentation entitled *Selection of the Optimal Personalized Treatment from Multiple Treatments with Multivariate Outcome Measures* at the Department of Mathematics & SimCenter Joint Colloquium Series on Friday, March 01, 2019. The speaker was fully funded along with an Honorarium of $1,0000 by the 2018/19 CEACSE Grant, SimCenter, UTC.

2. Prof. Margaret Wiecek from the School of Mathematical & Statistical Sciences at Clemson University, Clemson, SC, USA for a research presentation entitled *On Highly Robust Efficient Solutions to Uncertain Multiobjective Linear Programs* at the Department of Mathematics & SimCenter Joint Colloquium Series on Monday, April 08, 2019. The speaker was fully funded along with an Honorarium of $1,000 by the 2018/19 CEACSE Grant, SimCenter, UTC.

Challenges & Strategies Used to Address/Overcome:

- We are planning to develop data-driven statistical software that has the ability to create computer algorithms that process and statistically analyze massive amounts of biomedical data. This would enable designers in many industries to utilize and develop more advanced software systems to tackle mass or big data, make actions and decisions, e.g., discrimination of healthy from diseased with the aid of the univariate or multivariate Youden index and its corresponding cut-off value. This emerging data-intensive embedded computing paradigm brings a new set of data-induced challenges around guaranteeing timing predictability and tackling of missing, truncated, and censored data.
- Challenges that arise due to missing values can be tackled with the “imputation" process and censoring can be tackled with the cost-cutting techniques such as “grouping."

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

- Every aim outlined in the original proposal was achieved thanks to the teamwork of our research group.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

PI, Dr. Sumith Gunasekera, and CO-PI's, Drs. Lakmali Weerasena and Hong Qin, had greater opportunities

- to work in a research group of experienced and established researchers.
- to collaborate with experts in the interdisciplinary streams in- and out-side UTC.
- for high quality conference presentations, workshop participation, and to invite top-notch scholars for the research talks.
- to apply for external Federal Grants.
- to mentor doctoral, master's, and baccalaureate students for research works.
- to get the doctoral, master's, and baccalaureate students to be engaged in high-quality research work and grant writing, conference presentations, workshop participations.

- to seek and participate in conference/symposium/ colloquium/workshop/seminar opportunities.
- to explore deeper statistical and mathematical languages such as Python, R, SAS, MatLab, etc.
- to do collaborative scholarly and pedagogical works.
- to expedite tenure and promotions.

Students Impacted:

- Aruna Saram, Doctoral student in Computational Science with concentration in Computational and Applied Mathematics, July 2020, had greater opportunities to learn and explore new statistical and mathematical languages such as Python, R, SAS, MathLab, etc.

- Oluwakorede Ajumobi, Master's student, Mathematics with concentration in Statistics, May 2019, had greater opportunities to learn and explore new statistical and mathematical languages such as Python, R, SAS, MathLab, etc.

- Alissa Coleman, baccalaureate student, Engineering with concentration in Electrical Engineering, December 2020, had greater opportunities to learn and explore new statistical and mathematical languages such as Python, R, SAS, MathLab, etc.

- to work in a research group of experienced and established researchers.
- to learn how to read and write high quality research papers.
- to learn how to read and write high quality internal and external grants.
- to find the mentors for their respective dissertation and theses.
- to form their respective dissertation and thesis committees.
- to seek and participate in conference/symposium/ colloquium/workshop/seminar opportunities.
- to learn and explore new statistical and mathematical languages such as Python, R, SAS, MathLab, etc.
- to do collaborative scholarly and pedagogical works.
- to expedite their graduation in the hopes of embarking on to the next level of their career and future.

Community and Broader Impacts (Technical and Societal)

- The broader impact of the proposed research will mainly be the integration of research and education by advancing discovery and understanding while promoting teaching, training, and learning.
- The aim of the proposed study advances understanding both in the philosophy of medicine and in statistics itself through machine learning, which is an essential skill set to handle big data.
- Excel in machine learning has now become an essential part of the STEM (Science, Technology, Engineering, & Mathematics) education in this digitized era, and machine learning would be very useful in big data analysis and immensely prepare students for their future education and careers.
- This research will relate the workaday tools of the Youden index and the Receiver Operating Characteristic (ROC) curve to the broader, more abstract analysis of statistical inference.
- Such conceptual analysis is important in achieving pedagogically useful clarity of the basis, aims, and success of a discipline helpful to teaching, training, and learning with

the aid of machine learning-operated mass data analysis for both student research training and course adoptions.

- Professional statistics is hugely influential in the design and conduct of decision-making in every field.
- Opportunities for graduate and undergraduate research experiences, and in a suitable form it can used for outreach projects to incite the interest of high school children from under-represented groups.

Scholarly Products

- Software*:*

  Webservice framework called GeneralizedMultivariateYouden (GMY) builds modular high-performance computational resources that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers in the presence of missing and grouped, or pooled, data. GMY provides efficient data uploading and access and a suite of high computations on multivariate Youden index and its corresponding optimal cut-point, and Receiver Operating Characteristic (ROC) curve analysis code that can be used or adapted for any species, individuals, entities, or any electrical, electronic, or mechanical components. Code was written in Python and is supported by a relational database such as MySQL (Structured Query Language (SQL) named after one of the co-founder's daughter MY, an open-source rational database management system (RDBMS)) that incorporates the largest coherent collection of multivariate biomarkers (mBM) data.

- Publications*:*
  - Papers Published:

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

  - Papers in preparation:

Gunasekera, **S**., **Weerasena**, **L**., Saram, A. (2019). Exact Inference for the Multivariate Youden Index to Discriminate Individuals using Normally Distributed Samples.
Gunasekera, **S**., **Weerasena**, L., Saram, A. (2019). Exact Confidence Intervals for the Univariate Youden Index and Its Corresponding Optimal Cut-Point using Normally-, Mixture of Normally-, and t-Distributed Pooled Samples.

- External Conferences:

Gunasekera, S. 8th International Conference on Biostatistics & Bioinformatics (CB&B) sponsored by the Conference Series under the Theme *Exploring Advances in Biostatistics & Bioinformatics* from September 1617, 2019 in San Francisco, CA, USA.
Gunasekera, S. Estimating the Youden index under the multivariate ROC curve in the presence of missing values of mass diseased- and healthy-biomarker data, 2019
Gunasekera, S. 7th International Conference on Biostatistics & Bioinformatics (CB&B) sponsored by the Conference Series under the Theme *Exploring Advances in Biostatistics & Bioinformatics* held September 26–27, 2018 at Holiday Inn Chicago O 'Hare, Chicago, Illinois, USA.
Gunasekera, S. Exact inference for the Youden index to discriminate individuals using two-parameter exponentially distributed pooled samples, 2018
Gunasekera, S. Joint Statistical Meetings (JSM) sponsored jointly by the American Statistical Association (ASA), International Biometric Society (IBS) Eastern North American Region (ENAR), and Western North American Region (WNAR), Institute of Mathematical Statistics (IMS), Statistical Society of Canada (SSC), International Chinese Statistical Association (ICSA), International Indian Statistical Association (IISA), International Society for Bayesian Analysis (ISBA), Korean International Statistical Association (KISA), and Royal Statistical Society (RSS) under the Theme *Statistics: Making an Impact* from July 27–August 01, 2019 in Denver, Colorado, USA.
Gunasekera, S. . Bayesian inference for the common-location parameter of several shifted exponential populations, 2019
Wijekularathna, D. and Gunasekera, S. (2019). On Performing Generalized Inferences for the Burr XII Reliability Function based on Progressively Censored Data.

Scholarly and Pedagogical works at the Research Dialogues 2019 at UTC:
Gunasekera, **S**., **Weerasena**, **L**., Saram, A. Ajomobi Statistical Exploration of Stochastic Differential Equation Models used in the Stochastic Dynamics of Biological Systems: Statistical Algorithms & Computer Programs, 2019.
Gunasekera, **S**. Exact inference for the Youden index to discriminate individuals using two parameter exponentially distributed pooled samples. Podium Talk, 2018.
Gunasekera, **S**. Mathematics and Statistics: Who is the Winner? Faculty Elevator Pitch, 2019

- Preparation of*:*
    1. One (1) internal grant in CEACSE 2020/21.
    2. Four (4) External Grants in NSF-REU (Research Experience for Undergraduates) sponsored by the National Science Foundation (NSF), NSF-RUI (Research in Undergraduate Institutes) sponsored by the National Science Foundation (NSF), and NIH-R15-AREA (Academic Research Enhancement Award) or REAP (Research Enhancement Award) Programs sponsored by the National Institutes of Health (NIH), NIH/NSF-NIGMS/DMS grant opportunity by the National Institute of General Medical Science (NIGMS) of the National Institutes of Health (NIH) in collaboration with the Directorate of Mathematical Sciences (DMS) of the Division of Mathematical & Physical Sciences in the National Science Foundation (NSF) in collaboration with the UTC Faculty and Faculty from Troy University at Troy, Alabama, USA.
    3. Podium Talk, Panel Talk, Elevator Pitch Talk, Poster: Research Dialogues 2020

Research Outreach & Collaboration

- Invitation of:
    1. Prof. Karunarthna Kulasekera, Assistant Dean for Academic Affairs, School of Public Health and Information System, and Professor & Chair of the Department of Bioinformatics and Biostatistics at the University of Louisville, Louisville, Kentucky, USA, and former graduate coordinator in the Department of Mathematics & Statistics (presently School of Mathematical & Statistical Science) at Clemson University, for a research presentation entitled *Selection of the Optimal Personalized Treatment from Multiple Treatments with Multivariate Outcome Measures* at the Department of Mathematics & SimCenter. Joint Colloquium Series on Friday, March 01, 2019. The speaker was fully funded along with an Honorarium of $1,0000 by the 2018/19 CEACSE Grant, SimCenter, UTC.
    2. Prof. Margaret Wiecek from the School of Mathematical & Statistical Sciences at Clemson University, Clemson, SC, USA for a research presentation entitled *On Highly Robust Efficient Solutions to Uncertain Multiobjective Linear Programs* at the Department of Mathematics & SimCenter Joint Colloquium Series on Monday, April 08, 2019. The speaker was fully funded along with an Honorarium of $1,000 by the 2018/19 CEACSE Grant, SimCenter, UTC.

EXTERNAL FUNDING

Proposal Submissions
Four (4) External Grants in NSF-REU (Research Experience for Undergraduates) sponsored by the National Science Foundation (NSF), NSF-RUI (Research in Undergraduate Institutes) sponsored by the National Science Foundation (NSF), and NIH-R15-AREA (Academic Research Enhancement Award) or REAP (Research Enhancement Award) Programs

sponsored by the National Institutes of Health (NIH), NIH/NSF-NIGMS/DMS grant opportunity by the National Institute of General Medical Science (NIGMS) of the National Institutes of Health (NIH) in collaboration with the Directorate of Mathematical Sciences (DMS) of the Division of Mathematical & Physical Sciences in the National Science Foundation (NSF) in collaboration with the UTC Faculty and Faculty from Troy University at Troy, Alabama, USA

Sponsored Program Capacity Building Activities:
Mentoring of:

- Matthew McCarver, who secured a UTC URaCE (Undergraduate Research and Creative Endeavor) Summer REU (Research Experience for Undergraduate) for 2019.
- Emily Turner from Shippensburg University of Pennsylvania and Ashly Powell from the University of the Virgin Islands, who were selected for the NSF- (National Science Foundation) funded ICompBio: REU (Interdisciplinary Computational Biology Research Experience for Undergraduate) for Summer 2019.

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?
Extend the GeneralizedMultivariateYouden (GMY) that is useful in computing the generalized-variable-method-based multivariate Youden index to distinguish diseased from the healthy with several biomarkers. Regularly censor the data, including progressive censoring with fixed removals, progressive censoring with random removals, and truncated, ordered, and categorical data, etc.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?
Most of the other heavy and seminal research that are planned for the intended external grants opportunities.

Tell us anything else we should know about this work not described above.
Intent to extend the above-mentioned research in multivariate framework as well as in the vector filed and stochastic differential equations.

What barriers (if any) do you face to reach these next goals?
We would like to have our proposals funded every year, given that those proposals are excellent, so that we can easily achieve our research goals in larger scale and in depth. Our heartfelt thanks are always going to the Office of the VCR, Graduate School, CEACSE, SimCenter, and Department of Mathematics at UTC for their strong support for research and career building.

FINANCIAL ACCOUNTING

Funds were appropriately utilized for the success of the proposed project. We were awarded $97,901.00 and $95,416.16 was utilized with a remaining dollar amount of $2,484.84. Full budget report can be made available by me or can be accessed via Ms. Anna Lane (Multi-Disciplinary Research Building (MDRB), SimCenter, Dept. 7200, 701 E. ML King Blvd., Chattanooga, TN 37403, Phone: 423–425–5434, E-mail: Anna-Lane@utc.edu), Accounting Coordinator for the Vice Chancellor of Research & Dean of the Graduate School upon request.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Hope Klug, Lead PI

Co-PI(s): Jennifer Boyd, Azad Hossain, Hong Qin

Other Personnel: N/A

Project Title: "Using Computational Tools to Understand the Fundamental Rules of Life"

Date Submitted: 03/05/2018

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

We used big datasets, geographic information system (GIS) approaches, and computational tools to (1) develop and analyze biological networks (i.e., relationships) of interest across species and geospatial scales, (2) assess network robustness and stability, and (3) identify the key interactions that influence the genotype-phenotype map. We focused on three timely biological questions of interest: (1) What biological rules govern the expression of genes and how robust are gene/protein interactions? (2) Does phenotypic plasticity influence the relative abundance of species and what environmental factors and interactions influence plasticity? (3) What ecological, evolutionary, and behavioral interactions determine mating strategy and parental investment mode?

Our findings suggest that (1) aging increases noise in gene networks, but long-lived cells and calorie restriction are able to significantly suppress noise in the gene networks, which can be thought of as a "general rule" on aging regulation; (2) a variety of factors, including ecology, evolution, and development, likely influence whether species are rare versus common; and (3) a range of ecological factors, costs and benefits of alternative behaviors, and life-history traits can interact to influence the evolution of mating strategies and parental care. Additionally, our GIS research revealed that (4) imperiled plant and fish species are not randomly located across space but instead are potentially distributed non-randomly in relation to changes in environmental factors.

The proposed research involved substantial student training, led to (and will continue to lead to) multiple high-impact publications and papers in preparation, and contributed to or will serve as the foundation for multiple grant proposals.

PROJECT TITLE

Technology Area of Interest: Health and Biosystems

PROPOSED TECHNICAL APPROACH	OUTCOMES
Use big datasets, geographic information system (GIS) approaches, and computational tools to identify genetic, ecological, and evolutionary "rules of life." • Task 1: Use big datasets and network analysis to identify biological rules that govern the expression of genes and the robustness of gene/protein interactions; • Task 2: Use big datasets and network analysis to identify key factors that are expected, based on current research foci, to lead to rules of life that govern species rarity versus commonness; • Task 3: Use big datasets, network analysis, and mathematical modeling to identify the ecological, evolutionary, and behavioral interactions that determine mating strategy and parental investment mode; • Task 4: Incorporate geospatial tools into the above analyses and datasets to identify the environmental and geospatial factors that cause some species to be imperiled.	We identified the following biological 'rules of life'. Task 1: Permutation analyses revealed that aging increases noise in gene networks. Our findings also suggest that long-lived cells and calorie restriction can significantly suppress noise in gene networks. These findings suggests general rules on aging regulation in relation to gene networks. Task 2: Network analyses have begun to reveal the links between ecological, evolutionary, developmental, and abiotic factors in influencing plant rareness. This research will provide insight into the general rules that determine species abundance across biological and spatial scales. Task 3: Network analyses and simulations have revealed links between various life-history traits across large taxonomic scales. We also found general effects of life-history traits and ecology on the evolution of parental care and mating strategies, thus identifying several

evolutionary and behavioral rules of life.

Task 4: Using geospatial tools, we have identified the distribution of plant and fish species that range from “safe” to “extinct” in the United States. We have also identified the distribution of a range of environmental factors that will allow us to link species’ conservation status with changes in environmental parameters across spatial scales.

RESULTS

Our research revealed the following general results:

1. Aging can lead to noise or variation in gene networks, thus influencing phenotype (Figure 1).
2. Ecology, evolution, abiotic factors, and heterogeneity can influence species rareness (Figure 1).
3. Genes, ecology, heterogeneity, and abiotic factors can influence the evolution of parental care and mating phenotypes (Figure 1).
4. Geospatial and abiotic factors can influence species abundance and conservation status (Figure 1).

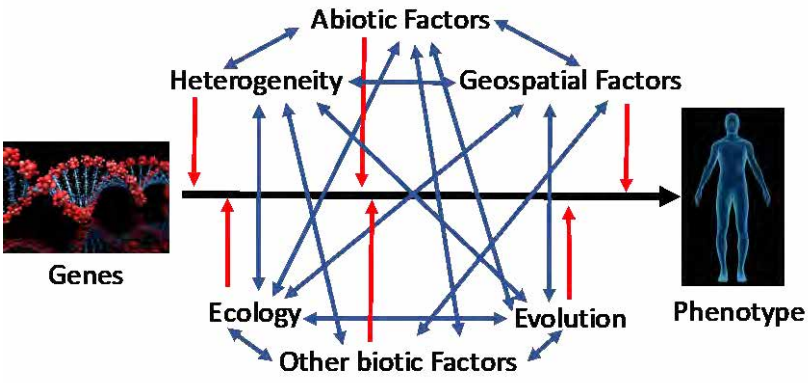


Figure 1. Factors that determine the rules of life, i.e., the rules that explain how given genes lead to given phenotypes. Ecology, evolution, other biotic factors, abiotic factors, heterogeneity, and geospatial factors can all directly (red arrows) influence the way in which genes code for aspects of

OTHER INFO

Budget and Schedule

Total Budget: $99,040.00

Actual Used: $95,856.12

Balance: $ 3,183.88

Total period of performance is 12 months.

Task 1: Months 1-12
Task 2: Months 1-12
Task 3: Months 1-12
Task 4: Months 1-3, 9-12

Deliverables

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

phenotype. However, these factors also interact with one another, and feedback is expected to occur among these factors (blue arrows).	• Publications • External and internal conference presentations **Organization Information** University of Tennessee at Chattanooga, 615 McCallie Avenue, Chattanooga, TN 37403

ACCOMPLISHMENTS & OUTCOMES

We used big datasets, geographic information system (GIS) approaches, and computational tools to (1) develop and analyze biological networks of interest across species and across geospatial scales, (2) assess network robustness and stability, and (3) identify the key interactions that influence the genotype→phenotype map. We focused on four biological questions of interest: (1) What biological rules govern the expression of genes and how robust are gene/protein interactions? (2) What drives species rarity and what is focused on in studies of species rarity? (3) What ecological, evolutionary, and behavioral interactions determine mating strategy and parental investment mode? (4) How are species distributed across the US in relation to conservation status and environmental parameters?

Predicting how genes and the environment interact to produce phenotypic traits is a fundamental question in the natural sciences, and recent research has revealed that the genotype-phenotype map is often complex. The research conducted as part of this grant has provided substantial insight into patterns of biological diversity across levels of biological organization and at various geographical scales. Specifically, the research completed thus far has allowed us to begin to identify general rules of life across scales in a range of organisms. We have found that: (1) aging increases noise in gene networks and that long-lived cells and calorie restriction can significantly suppress noise in gene networks; (2) a range of abiotic and biotic factors, including phenotypic plasticity, evolution, ecology, development, and environmental properties likely influence plant rarity and have been the focus of studies of plant rarity; (3) life-history traits are interconnected among species, and parental care and mating strategies can be influenced by costs and benefits of alternative behaviors and ecological factors; and (4) plant and fish abundance in relation to conservation status is variable across states in the US and potentially linked to a range of abiotic factors (e.g., temperature, precipitation).

Understanding how genotype is linked with phenotype and how phenotype is linked with abundance in relation to biotic and abiotic factors will have implications in relation to disease, agriculture, and species responses to global environmental change, and thus, our research is likely to have broad societal impacts.

In addition, the research facilitated the training of five undergraduate students and two graduate students in computational research. The research will allow for further novel collaborations among faculty with different expertise at UTC and broadened the expertise of all faculty and students involved.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop and analyze biological networks of interest across species and across geospatial scales	We developed and analyzed biological networks of interest in relation to rarity, abundance, life history, gene networks, and ecological and evolutionary dynamics across species.
Identify biological rules that govern the expression of genes and robustness of gene/protein interactions	We identified the following general rule: aging increases noise in gene networks and that long-lived cells and calorie restriction can significantly suppress noise in gene networks.
Identify drivers of species rarity	We identified a range of species that potentially influence plant rarity, including life history, ecology, evolution, and development. We additionally identified the geospatial distribution of plant and fish species across the US in relation to abiotic factors.
Identify ecological, evolutionary, and behavioral interactions that determine mating strategy and parental investment mode	We identified a range of factors that influence mating and parental strategies across species, including costs and benefits of each behavior, offspring need, adult and egg density, and life history.
Develop novel collaborations among faculty at UTC	We developed and expanded collaborations among faculty in Biology, Computer Science, and Geology. These collaborations will lead to future research.
Provide training and professional development opportunities for students	Seven students received hands-on training in computational biology.

Challenges & Strategies Used to Address / Overcome:
We encountered no major challenges in conducting our research. Minor challenges included the following: (1) coordinating novel, interdisciplinary research among four researchers in a relatively short time period (one year); and (2) pre-requisite issues prevented our MS in ESC graduate student from transferring to the Computational Science PhD program.

To overcome these challenges, we: (1) conducted substantial work during summer 2018 to ‘hit the ground running’; (2) trained students to extract, gather, and present large amounts of the data gathered; (3) developed plans to expand upon our collaborative research in the future; and

(4) encouraged our MS in ESC student to finish his MS degree prior to enrolling in the PhD program.

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

While we met all of our goals and objectives, there were some surprising and unexpected aspects of our research. First, we identified a major challenge associated with exploring the link between abiotic factors and the conservation status of species. Large, time-series datasets are available for abiotic factors through NASA, NOAA, etc. These datasets often provide monthly data for several decades on variables such as temperature and precipitation. However, data on species' conservation status and other biotic factors are typically only provided at a given, fixed point in time. Thus, correlating environmental change with changes in species' conservation status over time is challenging. Identifying this issue is an important finding, as it emphasizes the need for researchers to gather data on conservation status across varying timescales.

A second surprising outcome was the theoretical finding that in some cases, environmental factors can interact to create density-dependent offspring survival, which can in turn allow offspring abandonment and offspring consumption to function as forms of parental care. This finding was unexpected but has broadened our understanding of what we consider to be parental care. In general, our research also highlights the need for researchers to gather consistent ecological and evolutionary data.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The proposed research expanded the research programs of four faculty members from two departments and colleges. The research allowed biologists and geologists (Drs. Boyd, Klug, and Hossain) to collaborate with a computer scientist (Dr. Qin) and allowed for novel, biological, and geological research. The proposed research: (1) provided faculty and students with hands-on research experience; (2) created a novel alignment of faculty with different expertise and increase the research activity that is conducted at the SimCenter; and (3) allowed diverse students to participate in research activities at UTC.

Dr. Qin is a biologist and computer scientist with expertise in aging, genetics, and evolution. Dr. Qin has experience using computational approaches to study biological questions. Dr. Qin led the research associated with gene networks, and the CEACSE research expanded the biological and computational questions that Dr. Qin addresses.

Dr. Boyd is an ecologist with expertise in plant biology, global change biology, and linking ecological processes across multiple scales. Dr. Boyd has experience conducting field- and lab-based research. Dr. Boyd led the research associated with species rarity. The CEACSE research expanded Dr. Boyd's computational toolset and allowed her to address more complex biological questions.

Dr. Klug is an evolutionary biologist with expertise in life-history evolution and mating dynamics. Dr. Klug has experience conducting experimental research and using mathematical models in biology. Dr. Klug led the research associated with parental care and mating strategies. The CEACSE research expanded Dr. Klug's computational toolset and allowed her to address complex biological questions.

Dr. Hossain is a geologist with expertise in GIS, remote sensing, and spatial analysis. He has worked on several research projects that integrated geospatial technology with wide spectrum of computational models. Dr. Hossain provided GIS data and analyzed the data associated with the geospatial aspect of the project. The CEACSE research expanded Dr. Hossain's expertise in conservation biology in relation to geospatial variables.

Students Impacted

Richard Blanton, MS in Environmental Science in progress: Rick participated in all GIS components of the project.
Zachary McCoy, MS in Environmental Science in progress, plans to apply to PhD program once MS is complete: Zachary participated in ecological network research related to life history.
Jacob Burleson, BS in Geology in progress: Jacob participated in all GIS components of the project.
Braley Gentry, BS in Biology in progress: Braley participated in all aspects of the ecological network research.
Chelsea Langley, BS in Psychology 2018: Chelsea participated in ecological simulations related to parental care and mating strategies.
Zachary Sheckley, BS in Biology 2018: Zachary participated in data collection and ecological simulations related to fish life history, mating, and parental care.
Thomas Wiegand, BS in Biology in progress: Thomas participated in all aspects of the ecological network research.

Community and Broader Impacts

Understanding how genotypes link with phenotypes and how the genotype-phenotype map interacts with biotic and abiotic factors has implications in relation to disease, agriculture, and species responses to global environmental change. Our research findings (described above) will likely expand our understanding of factors that contribute to both aging and conservation, thus having societal implications. In addition, the research involved significant undergraduate and graduate student training. The PIs made it a priority to recruit students from diverse backgrounds.

Scholarly Products

Publications:

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

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

We anticipate additional manuscripts resulting from this research in the future.

External Conferences:

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H**, **Boyd J**. "Visualizing connectivity of ecological and evolutionary concepts with network analysis: an exploration of research on species rarity." Poster. World Congress on Undergraduate Research (WorldCUR); Carl Von Ossietzky Universität, Oldenburg, Germany, May 2019.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H**, **Boyd J**. "Visualizing connectivity of ecological and evolutionary concepts with network analysis: an exploration of research on species rarity." Poster. National Conference on Undergraduate Research (NCUR); Kennesaw State University, Kennesaw, GA, April 2019.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H**, **Boyd J.** "Visualizing connectivity of ecological and evolutionary concepts with network analysis: an exploration of research on species rarity." Poster. SoCon Undergraduate Research Forum (SURF); Wofford College, Spartanburg, SC, November 2018.

Klug, H. & Stone, L. "The role of chance in determining mating success" (Poster Presentation) Evolution 2018; Montpellier, August 2018.

Wiegand T, Gentry B, McCoy Z, Odell J, Odell H, Bonsall M, **Klug H, Boyd J.** "Visualizing connectivity of ecological and evolutionary concepts with network analysis." Poster. Ecological Society of America, New Orleans, LA, August 2018.

Hossain, **A**., Burleson, J., **Klug, H., Boyd, J**., and Blanton, R. "Developing a Geographic Information System to map and analyze the conservation status of conifers, ferns, and flowering plants in the United States," 12th Southeastern Forestry and Natural Resource management GIS Conference, December 9–10, 2019, Athens, GA.

Presentations at UTC:

1. Guo, H, **Qin**, **H**. "Network-based association study of protein sets and applications in gene ontology enrichment analysis." UTC Research Dialogues.
2. McCoy, Z. "Using big data to address questions in life-history evolution." UTC Research Dialogues.

Inventions or Other Intellectual Property

No new inventions or intellectual property resulted from this work.

Research Outreach & Collaboration

This research has facilitated and led to collaboration between Drs. Boyd, Hossain, Klug, and Qin. We expect these collaborations to continue and expand the computational research activities taking place at UTC.

In addition, this research has facilitated ongoing collaborations between Drs. Boyd and Klug and Dr. Mike Bonall (University of Oxford). These collaborations will also continue in the future and expand our computational research capabilities.

EXTERNAL FUNDING

Proposal Submissions

1. National Science Foundation, Division of Information & Intelligent Systems: Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education ($549,888) (Funded research team: P: H Qin; Co-PIs A Hossain, J Boyd, H Klug, and J Shaw; Note: Per the PO's request that some personnel be removed because there were an unusually large number of co-PIs on the overall collaborative grant, Boyd and Klug volunteered to be removed from this grant effective September 2018)
2. National Science Foundation, CC* Networking Infrastructure: Advancing high-speed networking at UTC for research and education. ($499,663 requested) (PI: F Kandah; Co-PIs: H Klug, A Skjellum, M Sartipi, D Gendron)
3. National Science Foundation, Major Research Instrumentation: Acquisition: A Research-as-a-Service (RaaS)-based Private Cloud for Innovative Science and Engineering ($921,109 requested) (PI: A Skjellum; Co-PIs: F Kandah, M Sartipi, H Klug, E Panagiotou)
4. NIH, R21, Using Permutations of Gene/Protein Networks for Pairwise Association Analysis of Genomic Data. Submitted in November 2018. Declined. PI: Qin.

Contracts/Awards Received

1. National Science Foundation, Division of Information & Intelligent Systems: Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education ($549,888) (Funded research team: P: H Qin; Co-PIs A Hossain, J Boyd, H Klug, and J Shaw; Note: Per the PO's request that some personnel be removed because there were an unusually large number of co-PIs on the overall collaborative grant, Boyd and Klug volunteered to be removed from this grant effective September 2018)
2. National Science Foundation, CC* Networking Infrastructure: Advancing high-speed networking at UTC for research and education. ($499,663 funded) (PI: F Kandah; Co-PIs: H Klug, A Skjellum, M Sartipi, D Gendron)

Sponsored Program Capacity Building Activities

1. All PIs actively wrote, managed, and planned for future grants during the award period.

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 1-3 years, we will follow up our CEACSE work with the following activities:

1) We have established geospatial maps of environmental variables over time in the US and species' conservation status for fish and plants in the US. In the future, we will link these maps to directly explore the relationship between environmental variables and species' conservation status. We will additionally broaden the scope of this research by expanding our analyses to include birds and mammals.
2) Continue our exploration of factors contributing to species rarity by using big data and computational tools.

3) Continue our exploration of factors influencing life-history evolution and the evolution of parental and mating strategies using big data and computational tools.
4) Continue using network analysis to explore aging.

In subsequent years, we anticipate submitting future NSF grants related to the three research foci described above.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?
The current research has increased Dr. Boyd and Klug's knowledge of how GIS tools can be used in ecological research. Likewise, the current research has increased Dr. Hossain's knowledge of how GIS tools can apply to conservation research. In the future, we expect additional research between the PIs focused on the integration of geospatial analyses in relation to conservation.

In addition, we expect to expand our research utilizing network analysis. This future research will continue to broaden and enhance our understanding of aging, species rarity, and the evolution of behavioral strategies.

Tell us anything else we should know about this work not described above.
The current research was transformative for the PI and Co-PI's research programs. While our previous CEACSE research allowed us to begin using network analysis to explore a range of pressing biological questions, the current research allowed us to both expand this research and incorporate geospatial tools into our research. We expect this grant to lead to funded research for all four PIs in the future.

What barriers (if any) do you face to reach these next goals?
In the future, it will be critical for us to find ongoing funding to support students to conduct the ongoing ecological/geospatial research that was spurred by the current CEACSE grant.

FINANCIAL ACCOUNTING

Remaining funds are due to difficulty in knowing what student and faculty benefit expenditures would be. In general, we could never get an accurate estimate of exactly what benefit charges would be associated with each students' pay for a given month, and this seems to be a general issue at UTC. In addition, because charges often didn't 'hit' our account until the following month, it was challenging, particularly near the end of the grant, to know exactly how much funding remained. Otherwise, we were regularly updated about the remaining funds in our grant, which was very helpful.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Lead PI Lingju Kong

Co-PI(s): John R. Graef and Andrew Ledoan

Project Title: “Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations”

Date Submitted: 07/30/2019

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

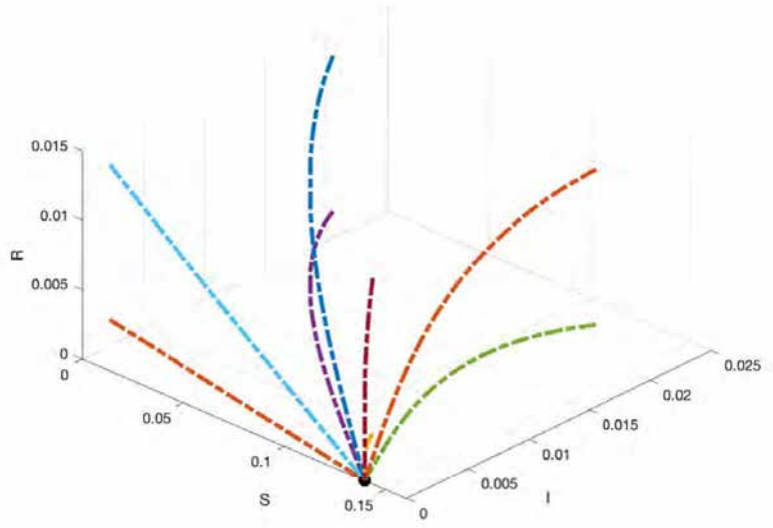
By drawing an analogy to the spreading dynamics of an infectious disease, we derive a fractional-order susceptible-infected-removed (SIR) model to examine the user adoption and abandonment of online social networks (OSNs), where adoption is analogous to infection and abandonment is analogous to recovery. We modify the traditional SIR model with demography, so that both infectious and noninfectious abandonment dynamics are incorporated into our model. More precisely, we consider two types of abandonments: infectious abandonment resulting from interactions between an abandoned and an adopted member and noninfectious abandonment without being influenced by an abandoned member. In addition, we study the existence and uniqueness of nonnegative solutions of the model, as well as the existence and stability of its equilibria. Our stability results show that the infectious abandonment dynamics does not contribute to the stability of the user-free and user-prevailing equilibria and that it only affects the location of the endemic equilibrium. The Jacobian matrix technique and the Lyapunov function method are used to show the stability of the equilibria. Numerical simulations are provided to verify these theoretical results.

This project demonstrates how to improve on previous studies by utilizing the theory of fractional calculus to supply a new and efficient approach for studying OSN dynamics. This project creates a framework in which the graduate student can more clearly understand the conceptual structure in which theoretical and numerical methods function as an aid to learning. Moreover, the research findings in this project may attract the interest of incumbent and emerging network providers and their stakeholders. This project aligns with the mission of the SimCenter of advancing modeling- and simulation-based science at UTC.

PROJECT TITLE

Modeling Online Social Network Dynamics and Predicting Information Diffusion with Fractional Differential Equations

PROPOSED TECHNICAL APPROACH	OUTCOMES
A fractional mathematical model is proposed and studied to analyze the dynamics of OSNs and extensive numerical simulations are performed to support the theoretical findings. Task 1: Collect/read relevant papers in the literature and derive the fractional model for OSNs. Task 2. Prove the existence and uniqueness of nonnegative solutions of the model. Task 3. Study the stability of the user-free equilibrium of the model. Task 4. Prove the existence of the user-prevailing equilibrium of the model and study its stability and the dependence of its location on the infectious abandonment rate. Task 5. Perform numerical simulations to confirm the theoretical findings. Task 6. Organize the obtained results in the form of a well-written paper.	We first construct a fractional-order epidemiological model to study user adoption and abandonment of an OSN, with adoption being analogous to infection and abandonment being analogous to recovery. Our model utilizes fractional-order ODEs and modifies the traditional susceptible-infected-removed (SIR) model with demography, so that it incorporates both infectious and noninfectious abandonment dynamics. We then discuss the existence and uniqueness of nonnegative solutions of the model and study the existence and stability of its equilibria. We utilize the Jacobian matrix technique and the Lyapunov function method to show the stability of the equilibria. Finally, we perform numerical simulations to illustrate our results.

RESULTS	OTHER INFO
1. Prove a theorem that guarantees the existence and uniqueness of nonnegative of solutions of the model and provides the positively invariant set of the model. 2. Prove two theorems on the locally asymptotically stability of the user-free equilibrium.  Fig. 1. Locally asymptotically stability of the user-free equilibrium. 3. Prove a theorem that guarantees the existence of the user-prevailing equilibrium. 4. Prove a theorem that guarantees the global stability of the user-prevailing equilibrium.	**Budget and Schedule** Total Budget: $96,380.00 Actual Used: $96,380.46 Balance: $ 0.00 Total period of performance is 12 months. Task 1: Months 1-2 Task 2: Months 3-4 Task 3: Months 5-6 Task 4: Months 7-9 Task 5: Months 10-11 Task 6: Months 11-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publications • External and internal conference presentation **Organization Information**

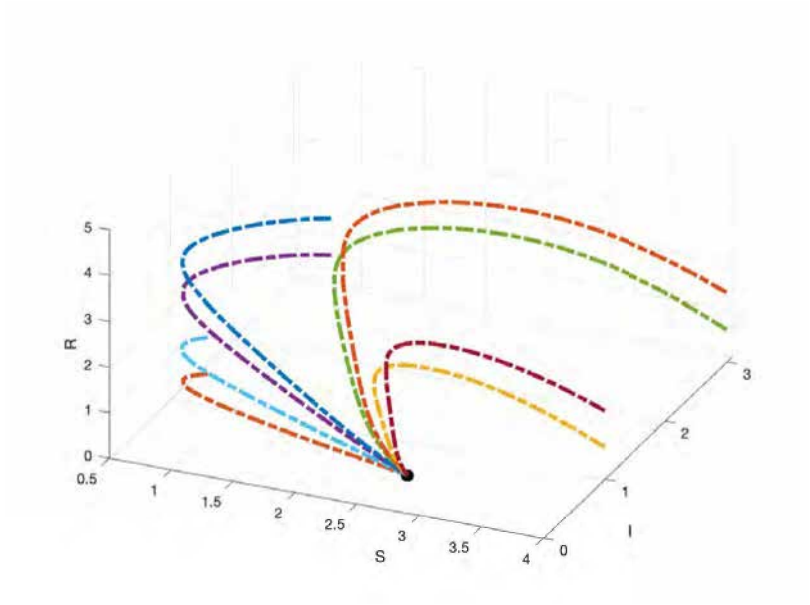


Fig 2. Globally asymptotically stability of the user-prevailing equilibrium.

5. Show how the location of the user-prevailing equilibrium depends on the infectious abandonment rate.

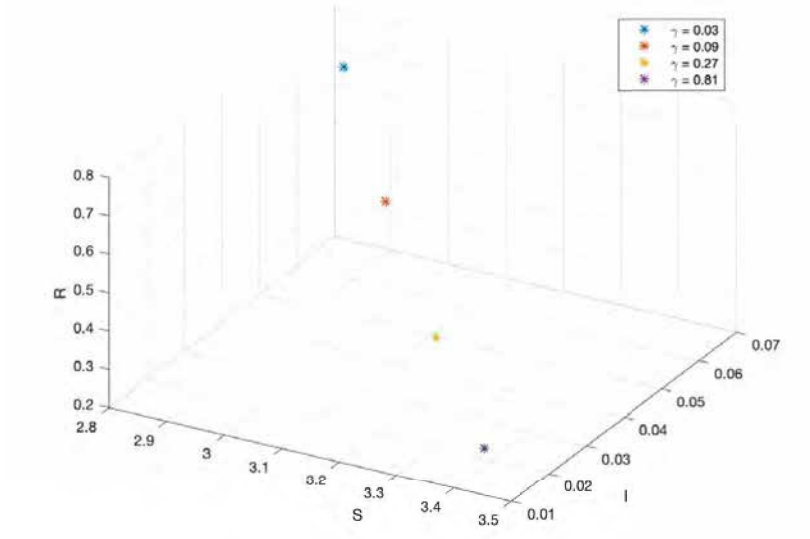


Fig. 3. Location of the user-prevailing equilibrium with respect to the abandonment rate.

6. investigate the impact of index of memory to the solution while other parameters are fixed.

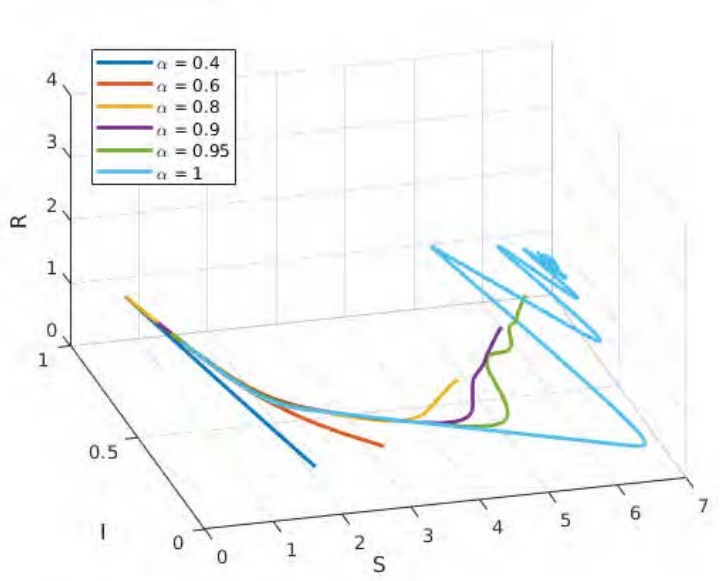


Fig. 4. Trajectories of the model with respect to the index of memory.

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
1. Derive a fractional mathematical model to study the dynamics of OSNs.	Achieved.
2. Establish the existence and uniqueness of nonnegative solutions of the model. This will ensure that the model is well-posed.	Achieved.
3. Establish the local stability of the user-free equilibrium of the model.	Achieved.
4. Prove the existence and uniqueness of user-prevailing equilibrium of the model.	Achieved.
5. Establish the global asymptotical stability of the model.	Achieved.

6. Perform numerical simulations to verify the theoretical findings.	Achieved.

Challenges & Strategies Used to Address / Overcome:

The project involves solving nontrivial problems. Many nontrivial analyses and original ideas are involved in this project and there are challenges at almost every stage of the project including formulating the model, proving the theorem, and performing the simulations. For instance, to prove the nonnegativity of solutions of the model and the global stability of the user-prevailing equilibrium of the model, the traditional techniques do not work because of the nonlocal nature of our model. New ideas and methodologies must be developed to address these challenges.

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

All the goals were achieved.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This project significantly impacts the PI and Co-PIs' research. The problem proposed in the project is a relatively new research area to us. During the process of completing the project, we read many related papers and learned many new ideas. Thus, this project will be very beneficial for our future research and professional growth, Moreover, the results from this project were presented at a professional meeting and will be published in a top refereed journal. This certainly gives international exposure to us, the Mathematics Department, and the University.

Students Impacted

Christopher Michael Corley the Ph.D. student was supported by this grant.

Community and Broader Impacts

This project integrates research and education by advancing discovery while promoting teaching, training, and learning. This project involves computational mathematics and differential equation analysis, ranging from method and algorithm development to error analysis and computer implementation. It provides an ideal opportunity for training graduate students and preparing them to do computational and applied mathematics research in the future. Research findings from the proposed activities have been presented at a professional meeting and will be published in scholarly journals and disseminated through future conference presentations and research seminars. Moreover, these research findings may attract the interest of incumbent and emerging network providers and their stakeholders.

Scholarly Products

Publications:

Work on each of the listed papers below was initiated during period of the CEACSE Grant. Support by the Grant is acknowledged in each of these papers.

1. S. Abbas, N. A. Arifi, M. Benchohra, and J. R. Graef, Random coupled systems of implicit Caputo-Hadamard fractional differential equations with multi-point boundary conditions in generalized Banach spaces, Dynamic Systems and Applications, 28 (2019), 329–350.
2. S. R. Grace, J. R. Graef, and E. Tunc, On the boundedness of nonoscillatory solutions of certain fractional differential equations with positive and negative terms, Applied Mathematics Letters 97 (2019), 114–120.
3. J. R. Graef, S. R. Grace, and E. Tunc, Oscillation criteria for even-order differential equations with unbounded neutral coefficients and distributed deviating arguments, Functional Differential Equations 25 (2018), 143–153.
4. J. R. Graef, S. R. Grace, and E. Tunc, Oscillatory behavior of third order nonlinear differential equations with a nonlinear nonpositive neutral term, Journal of Taibah University for Science 13 (2019), 704–710.
5. J. R. Graef, S. Heidarkhani, L. Kong, and A. Salari, Three weak solutions to a degenerate quasilinear elliptic system, Le Matematiche, LXXIV (2019), 191-210.
6. J. R. Graef, S. Ho, L. Kong, and M. Wang, A fractional differential equation model for bike share systems, Journal of Nonlinear Functional Analysis 2019 (2019), Article ID 23, 14pp.
7. L. Kong, A degenerate elliptic system with variable exponents, Science China Mathematics. 62 (2019), 1373–1390.
8. S. R. Grace and J. R. Graef, Oscillatory behavior of second order nonlinear difference equations with a nonlinear nonpositive neutral term, Miskolc Mathematical Notes, to appear.
9. S. R. Grace, J. R. Graef, and E. Tunc, On the asymptotic behavior of solutions of certain integro–differential equations, Journal of Applied Analysis and Computation, to appear.
10. J. R. Graef, S. R. Grace, and E. Tunc, Asymptotic behavior of solutions of higher order fractional differential equations with a Caputo-type Hadamard derivative, Progress in Fractional Differentiation and Applications, to appear.
11. N. Prabaharan, C. Dharuman, J. R. Graef, and E. Thandapani, New oscillation criteria for second order quasi-linear differential equations with a sub-linear neutral term, Applied Mathematics E-Notes, to appear.
12. S. Shokooh and J. R. Graef, Existence and multiplicity results for non-homogeneous Neumann problems in Orlicz-Sobolev spaces, Rendiconti del Circolo Matematico di Palermo Series 2, to appear.
13. A. Da, B. Hazarika, J. R. Graef, and R. P. Agarwal, Global attractivity of solution of functional nonlinear integral equations in two variables, submitted for publication.
14. A. Dogan and J. R. Graef, Existence of positive solutions to multi-point third order problems with sign changing nonlinearities, submitted for publication.
15. S. R. Grace, J. R. Graef, I. Jadlovska, Oscillatory behavior of second order nonlinear differential equations with mixed neutral terms, submitted for publication.
16. J. R. Graef, D. Beldjerd, and M. Remili, Some new stability, boundedness, and square integrability conditions for third order neutral delay differential equations, submitted for publication.
17. J. R. Graef, D. Beldjerd, and M. Remili, On stability, boundedness, and square integrability of solutions of certain third order neutral differential equations, submitted for publication.
18. J. R. Graef, S. R. Grace, and E. Tunc̦, Oscillation of even-order nonlinear differential equations with sublinear and superlinear neutral terms, submitted for publication.

19. J. R. Graef, L. Kong, S. Heidarkhani, and S. Moradi, Existence results for impulsive fractional differential equations with p-Laplacian via variational methods, submitted for publication.
20. J. R. Graef, L. Kong, A. Ledoan, and M. Wang, Modeling online social network dynamics using fractional-order epidemiological models, submitted for publication.
21. J. R. Graef, O. Ozdemir, A. Kaymaz, and E. Tunc, Oscillation of damped second order linear mixed neutral differential equations, submitted for publication.
22. J. R. Graef and B. Yang, Positive solutions of the complementary Lidstone boundary value problem, with B. Yang, submitted for publication.
23. A. M. Khatir, J. R. Graef, and M. Remili, Stability, boundedness, and square integrability of solutions to third order neutral differential equations with delay, submitted for publication.
24. S. Padhi, J. R.Graef, and A. Kanaujiya, Positive solutions to nonlinear elliptic equations depending on a parameter with Dirichlet boundary conditions, submitted for publication.
25. S. Abbas, N. A. Arifi, M. Benchohra, and J. R. Graef, Periodic mild solutions of infinite delay evolution equations with non-instantaneous impulses, submitted for publication.
26. C. Gugg and A. Ledoan, On a theorem of N. P. Romanoff, submitted for publication.
27. E. Eckels, S. Jin, A. Ledoan, and B. Tobin, Lower bounds for the L^1 norm of exponential sums, to be submitted.
28. S. Dhar and L. Kong, Multiple anti-periodic solutions for a difference equation of higher order, submitted for publication.
29. S. Dhar and L. Kong, Existence of multiple solutions for systems of fractional boundary value problems, to be submitted.

External Conferences:

1. On January 16, the PI has presented part of the results in the AMS Special Session on Fractional, Stochastic, and Hybrid Dynamical Systems with Applications, Joint Mathematics Meetings, Baltimore, MD, January 16–19, 2019.

The information of the Special session can be found via the link:

http://jointmathematicsmeetings.org/meetings/national/jmm2019/2217_program_ss19.html#title

The abstract of the presentation can be found via the link:

http://jointmathematicsmeetings.org/amsmtgs/2217_abstracts/1145-34-1763.pdf

2. The Ph.D. student, Christopher Michael Corley, attended the NSF-CBMS Conference: L-functions and Multiplicative Number Theory, in May 20–24, 2019, at University of Mississippi. The website for this conference is
https://math.olemiss.edu/cbms2019/

Christopher's purpose for going to the conference was to attend the ten lectures by Professor Kannan Soundararajan (Stanford) and to learn some new tools in the field. Since June 2019, Christopher and the Co-PI Dr. Andrew Ledoan have been working on a project in probability and mathematical statistics. It concerns the level curves of random polynomials and random sums. They are hoping to finish this project in the fall. Christopher plans to apply for an NSF Graduate Fellowship in the fall.

Presentations at UTC:

1. At the UTC annual Research Dialogue, the PI and Co-PIs had a poster titled "*Modeling online social network dynamics using fractional-order epidemiological models*".

Inventions or Other Intellectual Property

None

Research Outreach & Collaboration

As a result of this project, the PI and Co-PI had a pleasant collaboration with Dr. Min Wang from Kennesaw State University. We expect that this collaboration will continue in the future.

EXTERNAL FUNDING

Proposal Submissions

As a Co-PI, Dr. Lingju Kong, with Drs. Yu Liang and Dalei Wu from Computer Science and Engineering, has requested $495,380 from the National Science Foundation for the project entitled, "HDR I-DIRSE-FW: Collaborative Research: DSCE360 – A Data-driven Sustainable Community Ecosystem."

Contracts/Awards Received

None

Sponsored Program Capacity Building Activities

The PI and Co-PIs actively attended on-campus workshops.

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 near future, based on the work in the CEACSE grant, a proposal will be written and submitted to an appropriate agency.

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

An area closely related to the OSNs proposed in the CEACSE proposal is to study how information/rumor spreads in the networks. The PI plans to pursue this area of research in the future.

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

None

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

None

FINANCIAL ACCOUNTING

None.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Dr. Daniel Loveless, Lead PI

Co-PI(s): Dr. Don Reising
Other Personnel: Bharat Patel (M.S. student), Ahmed Ibrahim (M.S. student), Ryan Boggs (M.S. student), Artem Malashiy (UG student)

Project Title: Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications

Date Submitted: 08/26/2019

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

This program addressed several critical challenges posed by the increasing interest of using commercial off-the-shelf (COTS) hardware in space systems. The specific objectives were to (1) investigate radiation failure mechanisms in emerging electronics technologies and (2) explore techniques for improving the fault tolerance of COTS circuits and systems deployed in space environments. These objectives were accomplished through a comprehensive, coordinated modeling and experimental methodology using in situ measurement coupled with intelligent control using machine learning. Such an approach will close the gap in performance between strategic hardware and commercial hardware by leveraging the performance advantages offered by the latest technology nodes without the overhead required of radiation-hardening-by-design. This effort resulted in 4 international conference presentations, 1 journal publication, 1 additional journal submission, 1 additional conference submission, 1 grant funded by the Office of Naval Research, and 2 additional grant proposal submissions to the National Science Foundation (NSF) and National Reconnaissance Office (NRO). The project provided partial support to 3 graduate students and 1 undergraduate student.

This project supported the mission of the SimCenter by directly contributing both the Aerospace/Defense and Energy/Environment swimlanes. This research combined electronics device research with advanced computational modeling and simulation, resulting in an innovative concept with the potential to create a paradigm shift in electronics reliability assessment in space, defense, and commercial sectors.

Ionizing Radiation Effects Spectroscopy for Secure Space and Defense Communications

Technology Area of Interest: Aerospace and Defense / Energy and the Environment

PROPOSED TECHNICAL APPROACH	OUTCOMES
Two integrative research activities were crucial to satisfying the research objectives: (1) determine fundamental failure mechanisms in emerging COTS technologies and quantify statistical features with ionizing radiation effects spectroscopy (IRES), and (2) formulate a transformative radiation hardening strategy coupling in situ fault analysis through IRES and intelligent machine-learning-based control. The specific tasks were: • *(Task 1) Perform radiation effects measurements on advanced COTS devices (in support of activity 1)* • *(Task 2) Design radiation failure models (in support of activities 1 and 2)* • *(Task 3) Design a novel tool, Ionizing Radiation Effects Spectroscopy (IRES), for measuring the impact of such effects in operational communications systems (in support of activity 2)*	The proposed effort consists of the development of analytical and computational models and experimental work to describe radiation effects in emerging integrated circuit (IC) technologies, and the design of a generalized radiation hardening methodology. This project offered unique opportunities to develop in situ diagnostic measurement tools for radiation effects and reliability evaluation of devices and ICs. The techniques developed account for stochastic behavior and offer the potential for a paradigm shift in radiation hardening strategy. The resulting findings broaden our understanding of the fundamental mechanisms behind the disruptive trends in radiation performance and provide a basis for the development of methods for ensuring system reliability. This work offers a new approach to radiation mitigation and has the potential for transforming the way industry assesses electronic device, component, and system reliability. The stochastic methodology is technology agnostic and will allow for rapid expansion into emerging technologies. The research community is responding positively to the stated claims, as evident by our scholarly activity: 4 international conference presentations were given 3 different venues (2 with proceedings), 1 journal article is in review, 1 additional conference paper is in review, and 1 grant proposal was submitted and funded by the Office of Naval Research.

RESULTS	OTHER INFO
(Task 1) *Perform radiation measurements on advanced COTS devices (in support of activity 1).* This work used experimental measurements on a phase-locked loop (PLL) circuit fabricated in a 130 nm CMOS process [1][2] to demonstrate IRES for identification and analysis of single event transients (SETs). To facilitate the short 12-month period-of-performance and to mitigate risk associated with new device measurements, we leveraged a database of approximately 10,000 radiation effects measurements generated by the program's PI during his PhD studies. Simultaneously, this program allowed for the acquisition of new fast-transient measurement equipment, a high-performance photodiode, and a point radiation source for conducting a limited number of on-site radiation tests. Data were captured from two-photon absorption (TPA) laser experiments [2]-[6] on the PLL designed and fabricated in a 130 nm CMOS technology, available through the MOSIS foundry. The VCO has a center frequency (frequency at which $V_{inVCO}=V_{dd}/2$) and a maximum frequency of approximately 200 MHz and 530 MHz, respectively. The locking range of the PLL is between approximately 40 MHz and 350 MHz, over which the VCO is approximately linear with a gain of 7.75 GHz/V. SETs were injected into the PLL circuit using laser-induced carrier generation based on TPA using high peak power femtosecond pulses at sub-bandgap optical wavelengths [3]-[6]. The device under test (DUT) was mounted on a motorized xyz translation platform with 0.1 μm resolution. In TPA, optical pulses are focused through the backside of the wafer onto the front surface of the DUT with a 100× microscope objective, resulting in a near-Gaussian beam profile with an approximate diameter of 1.6 μm at focus [6]. Because the carrier deposition varies as the square of the irradiance (I2), this corresponds to a Gaussian carrier density distribution with an approximate diameter of 1.1 μm (full-width-at-half-maximum) [6]. This work presents data from a single incident laser energy for various operating frequencies within the PLL's linear operating region. A single incident energy was chosen in order to examine several aspects of the spectrographic analysis techniques discussed in the proceeding sections under control of constant energy transfer. All experiments were performed at room temperature with the nominal power supply voltage of 1.2 V. In order to characterize output transients following laser strikes within the PLL, a Tektronix-TDS5104 oscilloscope was used to capture output waveforms at the sample rate of 625 MS/s. The oscilloscope was set to trigger on the	**Budget and Schedule** Total Budget: $99,876.00 Actual Used: $92,609.68* Balance: $ 7,266.32* **Final ledger is still pending. This is an estimated value as travel has not appeared on ledger. The remaining balance is due to an overestimate of the Fringe Rates. All other line items are near $0.* Total period of performance is 12 months. Task 1: Months 9-12 Task 2: Months 7-12 Task 3: Months 1-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • **3 journal publications and conference proceedings (1 pending):** ◦ B. Patel, M. Joplin, R. C. Boggs, D. R. Reising, M. W. McCurdy, L. W. Massengill, and T. D. Loveless, "Ionizing Radiation Effects Spectroscopy for Analysis of Total-Ionizing Dose Degradation in RF Circuits," *IEEE Trans. Nucl. Sci.*, vol. 66, no. 1, pp. 61-68, Jan. 2019. ◦ T. D. Loveless, B. Patel, D. Reising, Senior Member, R. Roca, M. Allen, L. W. Massengill, and D. McMorrow, "Single Event Transient Spectroscopy," *in review, IEEE Trans. Nucl. Sci.,* Jan. 2020. ◦ R. Boggs, E. Richards, L. Massengill, and T. D. Loveless, "An Electro-Optical Simulation Methodology for the Analysis of

rising edge of the pulsed laser sync pulse, and the FastFrame feature was utilized to capture 10 transients per injection location. The experiment was performed by rasterizing the TPA laser through the CP sub-circuit at a step size of 0.2 μm. Figure 1 shows an example SET following a laser perturbation at the CP output node. Following the laser strike, the output frequency (fout) was reduced to approximately 50 MHz, increasing the phase displacement (ϕout) to approximately 15 radians. The recovery time of the PLL was over 200 ns, corresponding to the PLL's initial lock time, indicating near-complete depletion of the charge stored on CLPF.

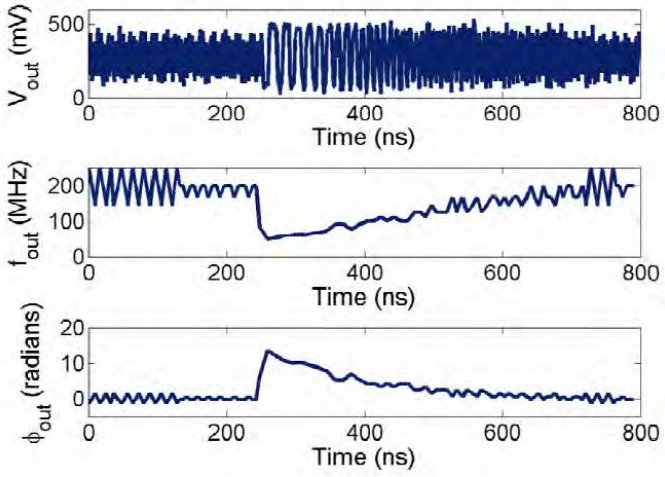


Fig. 1. Example of an output transient following a laser perturbation in the CP sub-circuit of the 130 nm PLL. The PLL was operating at 200 MHz prior to the laser strike. Following the laser strike, the output frequency was reduced to approximately 50 MHz, thus increasing the output phase displacement to approximately 15 radians. The recovery time of the PLL was over 200 ns [2].

Figure 2 illustrates a two-dimensional (2D) spatial map of the sensitive regions in the CP sub-circuit. Each pixel in the figure represents the average maximum phase displacement (instantaneous cycle-to-cycle phase error) for ten SETs generated at each x-y location [6]. The image illustrates that the output of the CP circuit, in particular the NMOS switches and current sources contain the most sensitive junctions due to their ability to deplete the charge stored in CLPF. The following sections employ various spectrographic analysis techniques for identification and quantification of these transients. Short-time windowed spectroscopy techniques, in particular the statistics-based method presented herein, allows for detailed examination of transient phenomena with low computational overhead. The techniques are especially useful when analyzing noisy data.

Single-Event Radiation Effects in Photonic Devices," proceedings of the 2019 IEEE SoutheastCon, Huntsville, AL, Mar. 2019.

- **5 External conference presentations (1 pending)**
  - T. D. Loveless, B. Patel, D. Reising, Senior Member, R. Roca, M. Allen, L. W. Massengill, and D. McMorrow, "Single Event Transient Analysis of RF Circuits via Ionizing Radiation Effects Spectroscopy," IEEE Nuclear and Space Radiation Effects Conference, PB-2, San Antonio, TX, July 2019.
  - B. Patel, D. Reising, L. W. Massengill, and T. D. Loveless, "Single Event Transient Analysis via Ionizing Radiation Effects Spectroscopy," presented at the 2019 Single Event Effects Symposium, La Jolla, CA, April 2019.
  - R. Boggs, E. Richards, L. Massengill, and T. D. Loveless, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," presented at the 2019 Single Event Effects Symposium, La Jolla, CA, April 2019.
  - R. Boggs, E. Richards, L. Massengill, and T. D. Loveless, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," presented at the 2019 IEEE SoutheastCon, Huntsville, AL, Mar. 2019.
  - A. Ibrahim, B. Mitchell, K. Hall, D. Reising, and T. D. Loveless, "The Effects of a Phase Modulated Clock and Temperature on RF-DNA Fingerprints in IEEE 802.11a Wi-Fi Signals," *submitted to the*

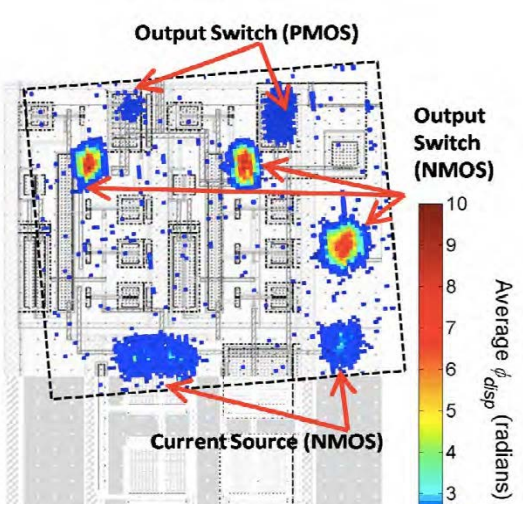


Fig. 2. A two-dimensional (2D) spatial map of the regions in the CP sub-circuit sensitive to SETs. The experiment was performed using laser TPA at a step size of 0.2 µm. Each pixel represents the average maximum phase displacement (instantaneous cycle-to-cycle phase error) for 10 SETs generated at each x-y location. The image illustrates that the output of the CP circuit, in particular the NMOS switches and current sources contain the most sensitive junctions due to their ability to deplete the charge stored in C_{LPF} (after [2]).

(Task 2) Design radiation failure models (in support of activities 1 and 2).

Simulations were performed using a behavioral model to approximate the PLL as a linear system with the ideal design parameters provided in [2]. The PLL model was designed with Verilog-A to match the circuit dynamics of the DUT used for experimental validation. SET simulations were performed with the Cadence Spectre circuit simulator. Reference [2] showed that the SET response of the PLL circuit is dominated by the loop parameters, is largely independent of the ion strike time constants, and is proportional to the deposited charge. Equation (1) shows the expected voltage perturbation (V_e) at the VCO's control voltage versus deposited charge Q_{SET} and the initial transient pulse width t_{SET}.

$$V_e = \frac{Q_{SET}+I_{CP}t_{SET}}{C_{LPF}} \cong \frac{Q_{SET}}{C_{LPF}} \quad (1)$$

In (1), I_{CP} is the PLL's charge pump current and C_{LPF} is the capacitance of the dominant pole in the loop filter. In general, the quantity $I_{CP}\times t_{SET}$ will be much smaller than Q_{SET} due to the short SET pulse widths in modern CMOS. Thus, a double exponential model for the ion strike was used to create the initial loop perturbation, rather than a more accurate ion strike model. The transient curves for various levels of deposited charge (determined by integrating the ion strike current pulse) are provided in Fig. 3 where the VCO control node (V_{inVCO}) versus time following simulated ion strikes to NMOS transistors at the output of the CP sub circuit at 260 MHz are provided. Note that this node is internal to the PLL loop and may not be accessible experimentally. Given a linear VCO, V_{inVCO} is

2020 IEEE Radio and Wireless Symposium (RWS2020).

- **5 Internal conference presentations**
  - R. Boggs, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," 2019 UTC Research Dialogues.
  - B. Patel, "Ionizing Radiation Effects Spectroscopy," 2019 UTC Research Dialogues.
  - A. Ibrahim, "Unlocking the Secrets of RF-DNA Fingerprinting," 2019 UTC Research Dialogues.
  - Artem Malashiy, "The UTChattSat Small-Satellite Platform," *presented at the 2019 Research Dialogues, UTC*, Apr. 2019.
  - R. Boggs, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," 2019 CECS Technology Symposium.
  - A. Ibrahim, "Unlocking the Secrets of RF-DNA Fingerprinting," 2019 CECS Technology Symposium.

Organization Information

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proportional to the PLL's output frequency and is an indicator of the current state of the loop. As expected, the voltage perturbation and recovery time of the PLL increase as the deposited charge increases. These changes in the recovery time and control voltage are gauges of the deposited charge and indicate a representative behavioral model. These simulation results are consistent with other works and indicate adequate loop dynamics for capturing SET phenomena.

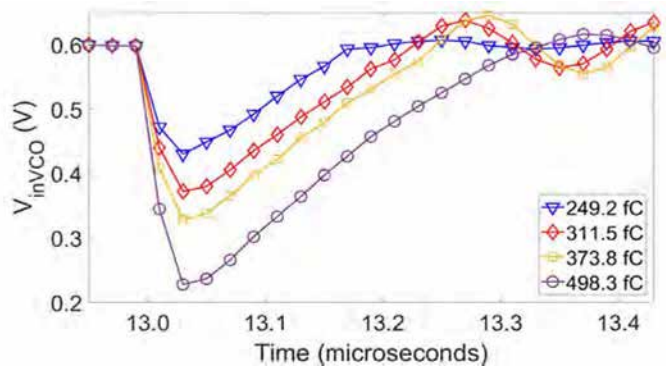

Fig. 3. Simulated ion strikes to NMOS transistors at output of the CP after various levels of charge deposited from a current source. These results show a recovery times between 200 and 300 ns and voltage perturbations between 0.15 and 0.4 V.

(Task 3) Design a novel tool, Ionizing Radiation Effects Spectroscopy (IRES), for measuring the impact of such effects in operational communications systems (in support of activity 2)

Ionizing radiation effects spectroscopy (IRES) is a method to augment time-frequency analysis through the statistical measurement of the waveform dynamics. This type of analysis is intended to leverage the computational savings achieved with windowed filtering while providing a simple methodology for quantifying detected events. IRES is based on Radio Frequency-Distinct Native Attribute (RF-DNA) fingerprinting for the identification of essential statistical features of erroneous signals within a device, circuit, or system. RF-DNA fingerprinting is a waveform-based technique used for augmenting existing wireless network security mechanisms. RF-DNA fingerprinting can be employed in the 1D time or frequency domains, or in 2D through time-frequency analysis. Works have demonstrated successes in the use of RF-DNA for identification of unique serial numbers from parts manufactured by the same vendor and containing the same model number [7]. Similarly, IRES uses key statistical measures of arbitrary signals within a device, circuit, or system for correlation to radiation vulnerabilities. IRES was first demonstrated in [8] to determine the operational bias voltage and total-ionizing dose (TID) exposure level in RF circuits. IRES images show shifting stochastic behavior with increasing TID

levels that are unique for each operational state. These unique states allow for machine-learning models to identify and quantify degradation amidst variation in operational conditions.

In this work, the IRES technique is applied to time-domain signals such that SETs can be identified through statistical measurements of *L* signal metrics (e.g., cycle-to-mean jitter and instantaneous frequency). Similar to the time-frequency analysis, IRES modulates an arbitrary

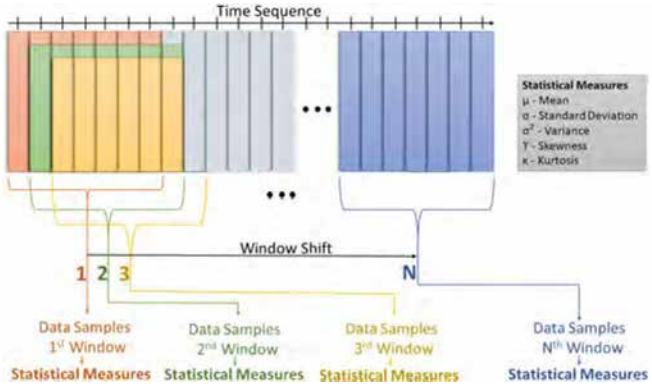

Fig. 4. Illustration of the window sampling method used for the calculation of statistical measures used in IRES.

waveform with a window function. Data within the windows are then viewed from a statistical point of view in order to (i) assess the likelihood of SET behavior within a window and (ii) quantify the severity of detected SETs. The use of multi-dimensional statistical analysis allows for easier identification of spurious transients in the presence of noise and allows for ease of integration with statistical models, when compared to standard measurement approaches. The technique naturally accounts for variability due to process and measurement uncertainty. IRES images are shown to capture inherent radiation effects mechanisms and the resulting impact on circuit behavior.

Figure 4 illustrates the window sampling process where statistical measures are computed for each window. The statistical measures may include the mean, standard deviation, variance, skewness, and kurtosis of an arbitrary signal. In this case, we perform the statistical sampling on the cycle-to-mean jitter feature due to the improved noise performance and low data rate requirement. The mean of the instantaneous output frequency is also calculated for each window for a visual of the transient in a traditional form and for comparison to spectrograms. Once the statistical measures are computed within each window and normalized such that the maximum value of any measure is 1, they are concatenated to form a column vector. These column vectors are arranged as a pseudo time-sequence, forming an IRES image of the SET characteristic behavior.

Figure 5 shows the (a) unfiltered and (b) filtered IRES images of an experimentally measured SET generated from a laser strike to an NMOS transistor at the output node of the CP within the PLL operating at ~150 MHz. Skew and Kur of the cycle-to-mean jitter indicate the start

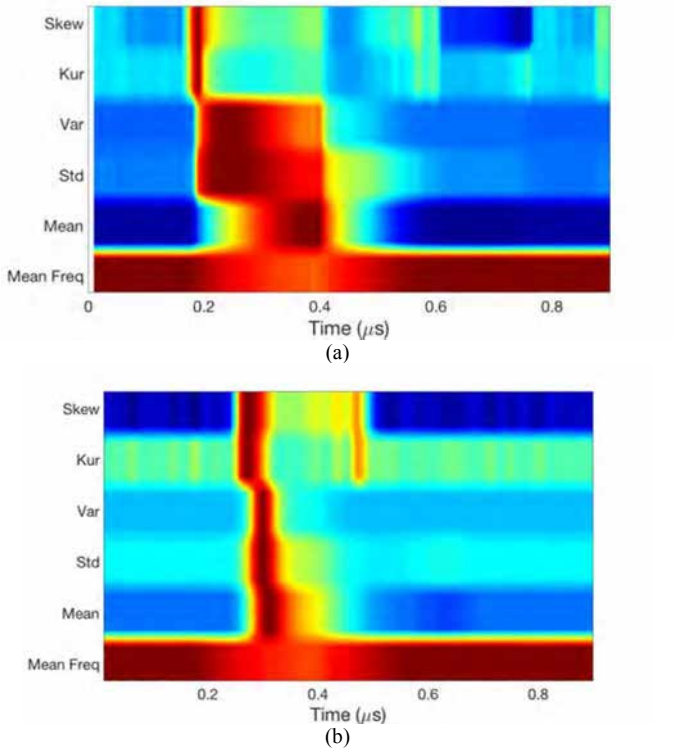

Fig. 5. IRES images of an experimentally measured SET originating from a strike on an NMOS transistor connected to the output node of the CP within the PLL operating at ~150 MHz. Six statistical measures were computed within a sliding window sized to 20% of the total sample space and shifted by 1 sample (95% overlap). The spectrograms were computed with (a) rectangular and (b) Gaussian filters. Peaks in skewness and kurtosis of the cycle-to-mean jitter indicate the start of the SET. The statistical measures of the cycle-to-mean jitter are used to identify radiation and circuit response mechanisms.

of the SET. The statistical measures of the cycle-to-mean jitter are used to identify radiation and circuit response mechanisms. The IRES image indicates that the statistical features are unique to the response signature. Moreover, the experimentally obtained signatures match the predicted images generated from simulations. Further, the normalization used to create the IRES images allows for removal of the magnitude of the ion strike, thus creating a “fingerprint” characteristic of the origins of the ion strike. These characteristic IRES features appear to be inherent to the circuit, the location of the strike, and the charge collection mechanisms.

Further, the use of multi-dimensional statistical analysis allows for identification of spurious transients in the presence of noise and for integration with statistical models. This is illustrated through the use of data

captured from TPA laser experiments on a PLL designed and fabricated in a 130 nm CMOS technology, and further illustrated through the use of behavioral modeling of the circuit dynamics. IRES shows that SETs can be detected through statistical analysis of waveform behavior rather than standard signal measurement, allowing for the capture of the subtle changes in loop recovery time as well as charge dynamics. The technique leverages computational benefits of windowed joint time-frequency analysis, requiring as little as 0.2% of the data samples required in high-resolution DFT analysis, while providing a statistical method for accurately estimating the SET characteristics, such as magnitude and pulse width.

NOTE: This work supported two additional tasks (not included in the original statement of work). These tasks were:

1) Development of an Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices. Here, the radiation effects modeling work platforms developed in this work was applied to photonic devices.

2) The Effects of a Phase Modulated Clock and Temperature on RF-DNA Fingerprints in IEEE 802.11a Wi-Fi Signals. Here, RF-DNA and IRES were applied to software defined radio transceivers configured for IEEE 802.11a. GNU Radio, the LimeSDR, and the HackRF One SDR platforms were used to design and implement WiFi transceivers, apply the latest RF-DNA and IRES research to analyze the behavior, and determine the influence of external and internal manipulation of the signatures.

References:

[1] T. D. Loveless, L. W. Massengill, W. T. Holman, and B. L. Bhuva, “Modeling and Mitigating Single-Event Transients in Voltage-Controlled Oscillators,” IEEE Trans. Nucl. Sci., vol. 54, no. 6, pp. 2561-2567, Dec. 2007.

[2] T. Daniel Loveless, Lloyd W. Massengill, W. Timothy Holman, Bharat L. Bhuva, Dale McMorrow, and J. Warner, “A Generalized Linear Model for Single Event Transient Propagation in Phase-Locked Loops,” IEEE Trans. Nucl. Sci., vol. 57, no. 5, pp. 2933-2947, Oct. 2010.

[3] D. McMorrow, W. T. Lotshaw, J. S. Melinger, S. Buchner, Y. Boulghassoul, L. W. Massengill, and R. L. Pease, “Three-dimensional mapping of single-event effects using two photon absorption,” IEEE Trans. Nucl. Sci., vol. 50, pp. 2199–2207, 2003.

[4] D. McMorrow, W. T. Lotshaw, J. S. Melinger, S. Buchner, and R. L. Pease, “Subbandgap laser-induced single event effects: Carrier generation via two-photon absorption,” IEEE Trans. Nucl. Sci., vol. 49, pp. 3002–3008, 2002.

[5] E. W. Van Stryland, H. Vanherzeele, M. A. Woodall, M. J. Soileau, A. L. Smirl, S. Guha, and T. F. Boggess, “Two photon absorption, nonlinear refraction and optical limiting,” Opt. Eng., vol. 24, pp. 613–623, 1985.

[6] T. F. Boggess, K. M. Bohnert, K. Mansour, S. C. Moss, I. W. Boyd, and A. L. Smirl, “Simultaneous measurement of the two-photon coefficient and free-carrier cross section above the bandgap of crystalline silicon,” IEEE J. Quant. Elect., vol. 22, pp. 360–368, 1986.

[7] C. Wheeler*, and D. 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.

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

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments

Determine fundamental failure mechanisms in emerging COTS technologies and quantify the statistical features with IRES	• Radiation effects testing data using laser two-photon absorption on phase-locked loop (PLL) circuits fabricated in a 130 nm CMOS technology were used to demonstrate IRES technique. Outcomes:
	  ○ Developed a novel transient anomaly characterization methodology
	  ○ 2 conference presentations at the 2019 SEE Symposium (Apr 2019) and 2019 IEEE NSREC (July 2019)
	  ○ 1 journal paper submitted to IEEE Transactions on Nuclear Science in review
	  ○ 1 M.S. student scheduled to graduate in December 2019
	• A Wi-Fi transceiver was designed using GNUradio for programming in commercially available LimeSDR and HackRF One software-defined-radio platforms. Outcomes:
	  ○ Integrates simulation and experimental methodologies for evaluation of extreme environment effects in complex architectures
	  ○ Allowed for discovery of thermal and radiation effects in RF transceivers
	  ○ 1 conference paper submitted to RWW2020 and currently in review
	  ○ M.S. graduate student received SEARCH award
	  ○ 1 M.S. student scheduled to graduate in December 2019
	• A three-dimensional tool flow was designed for simulation of radiation effects in photonic integrated circuits. Outcomes:
	  ○ Methodology demonstrated for co-simulation of optical and electrical domains
	  ○ Discovered potential mechanisms of transient effects in optical waveguides
	  ○ 2 conference presentations at the 2019 IEEE SoutheastCon and 2019 SEE Symposium
	  ○ 1 conference proceedings paper (IEEE SoutheastCon)
	  ○ 1 M.S. student graduated in August 2019

Formulate a radiation hardening strategy coupling in situ fault analysis through IRES and machine-learning-based control	• IRES signatures are shown to be unique to the origin of the radiation-induced transient • A behavioral model (designed using the Verilog-A hardware description language) was developed to match the electrical characteristics of the 130 nm PLL. Simulated IRES signatures match experimentally observed signatures. • IRES was analyzed and observed to reduce computational requirements when compared to standard spectral techniques by over 99% • Novel radiation hardening strategy was conceptualized and used to support 2 proposal submissions to ONR and NRO (1 proposal awarded and 1 still pending)

Challenges & Strategies Used to Address / Overcome:

There were several moving parts to our program including: device acquisition and measurement, experiment design, model development, simulation studies, and system design and test. We leveraged several additional students over what was originally planned in order to parallelize our task structure. Further, we redesigned the experimental efforts in order to leverage existing data sets. This allowed us to focus on modeling and simulation work. All experimental efforts were then directed to the system (software-defined radio), rather than depending on early experiments, allowing our analysis techniques to mature. Specifically,

1) We experienced a small delay in simulation work due to a delay in a software license renewal. This was resolved within the first several months of the program.

2) Device Procurement: We experienced several delays in device procurement, as this relied on collaboration with partners at Sandia National Labs. However, we refocused the effort to leverage data samples we already had. These measurements agreed with behavioral models developed in this effort and were therefore used to replace the originally planned device measurements. This ended up resulting in a powerful story supported by an extensive data set, behavioral models, and novel analyses.

3) SDR Design: We experienced several issues decoding data transmitted over a wireless path enabled by the developed SDR transceiver. This was mitigated by limiting the analysis to intact Wi-Fi preambles to establish baseline RF-DNA fingerprints.

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

We realized early in the program that we would not be successful if we depended on new device acquisition and measurement. Therefore, we removed all dependencies and leveraged existing data sets. This allowed us to proceed and develop the novel approaches we proposed. This program was wildly successful, resulting in several presentations, publications, and a newly funded grant.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

D. Loveless: This effort has resulted in 4 international conference presentations, 1 journal publication, 1 additional journal submission, 1 additional conference submission, 1 grant funded by the Office of Naval Research, and 2 additional grant proposal submissions to the National Science Foundation (NSF) and National Reconnaissance Office (NRO) and represents a significant advancement in Dr. Loveless' established Reliable Electronics and Systems (RES) laboratory at UTC. This work has resulted in increased the RES lab credibility and Dr. Loveless' career as a whole; Dr. Loveless was recently recognized as the recipient of the inaugural 2019 IEEE Nuclear and Plasma Science Society's Radiation Effects Early Achievement Award. Findings from this grant, and recent international recognition has the potential for generating several new collaborations with the University of Washington, Georgia Tech, and the Naval Research Laboratory.

D. Reising: This grant has led to 3 paper submissions (1 accepted, 2 under review) that will be part of Dr. Reising's promotion and tenure package this year. It has led to one funded grant award (ONR) and another grant proposal submission (NRO). This work will also be leveraged in an NSF SaTC submission with Drs. Skjellum, Kandah, and Loveless. It has stimulated the integration of IRES within the RF-DNA fingerprinting process to pull-out "hidden" and intentionally inserted features. It has led Dr. Reising and Dr. Loveless to

create a novel approach to performing in-situ electronics reliability assessment within austere (radiation, temperature) environments, which presents a significant shift to the current state-of-the-art.

Students Impacted

Ryan Boggs: This work partially supported Ryan as an M.S. student in Electrical Engineering. Ryan presented his CEACSE-funded work on photonic device modeling and simulation at 2 conferences, one of which resulted in a published proceeding. Ryan graduated in August 2019.

Ahmed Ibrahim: This work supported Ahmed as an M.S. student in Electrical Engineering. Ahmed submitted 1 paper to a refereed conference regarding this effort (still pending). He was the recipient of a UTC SEARCH award to supplement his efforts and to acquire additional hardware for demonstration of his Wi-Fi transceiver at the focus of his work. Ahmed plans to graduate in December 2019.

Artem Malashiy: Artem Malashiy was supported as an Undergraduate Research Assistant throughout this CEACSE effort. Artem graduated in May 2019.

Bharat Patel: This work supported Bharat as an M.S. student in Electrical Engineering. Bharat presented his CEACSE-funded work on the IRES technique at 2 conferences and submitted 1 paper to a refereed journal regarding this effort (still pending). Bharat plans to graduate in December 2019.

Community and Broader Impacts

The space and radiation effects industries are beginning to take note of our lab's work product, as several new requests for interns and full-time employees have been received over the past several months. This work has acted like a catalyst to new collaboration, is helping recruit, and is reaching the broader technical community. Further, research conducted in this program was leveraged for the past summer's NSF-funded REU program focused on undergraduate research.

Scholarly Products

Journal Publications:

1. T. D. Loveless, B. Patel, D. Reising, R. Roca, M. Allen, L. W. Massengill, and D. McMorrow, "Single Event Transient Spectroscopy," *in review*, *IEEE Trans. Nucl. Sci.*, Jan 2020.
2. B. Patel, M. Joplin, R. C. Boggs, D. R. Reising, M. W. McCurdy, L. W. Massengill, and T. D. Loveless, "Ionizing Radiation Effects Spectroscopy for Analysis of Total-Ionizing Dose Degradation in RF Circuits," *IEEE Trans. Nucl. Sci.*, vol. 66, no. 1, pp. 61-68, Jan. 2019.

Refereed Conference Proceedings:

1. A. Ibrahim, W. Mitchell, K. Hall, D. Reising, and D. Loveless, "The Effects of a Phase Modulated Clock and Temperature on RF-DNA Fingerprints in IEEE 802.11a Wi-Fi Signals," *in review*, Radio and Wireless Symposium (RWS2020), Jan. 2020.
2. T. D. Loveless, B. Patel, D. Reising, and L. W. Massengill, "Spectrographic Analysis of Single Event Transients in RF Circuits," *2019 IEEE Nuclear and Space Radiation Effects Conference (NSREC)*, paper B-2, San Antonio, TX, July 2019.
3. R. C. Boggs, E. Richards, L. W. Massengill, and T. D. Loveless, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," *2019 IEEE Southeast Conference*, Apr. 2019.

Non-Refereed Conference Proceedings:

1. R. C. Boggs, E. Richards, L. W. Massengill, and T. D. Loveless, "An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices," *2019 Single Event Effects Symposium*, May 2019.

2. B. Patel, D. Reising, L. W. Massengill, and T. D. Loveless, “Single Event Transient Analysis with Ionizing Radiation Effects Spectroscopy (IRES),” *2019 Single Event Effects Symposium*, May 2019.

Presentations at UTC:

1. Ahmed Ibrahim, “Unlocking the Secrets of RF-DNA Fingerprinting,” *presented at the 2019 Research Dialogues, UTC*, Apr. 2019.
2. Bharat Patel, “Single Event Transient Analysis with Ionizing Radiation Effects Spectroscopy,” *presented at the 2019 Research Dialogues, UTC*, Apr. 2019.
3. Artem Malashiy, “The UTChattSat Small-Satellite Platform,” *presented at the 2019 Research Dialogues, UTC*, Apr. 2019.
4. R. Boggs, “An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices,” 2019 UTC Research Dialogues.
5. R. Boggs, “An Electro-Optical Simulation Methodology for the Analysis of Single-Event Radiation Effects in Photonic Devices,” 2019 CECS Technology Symposium.
6. A. Ibrahim, “Unlocking the Secrets of RF-DNA Fingerprinting,” 2019 CECS Technology Symposium.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

This work resulted in a ***new*** collaboration with Dr. Dale McMorrow (recently awarded *IEEE Fellow Grade*) at the Naval Research Laboratory. Dr. McMorrow was a collaborator on our publication submitted to the IEEE Transactions on Nuclear Science. We are currently planning future experiments in his laser laboratory.

We also ***expect new*** collaborations with Dr. John Cressler at Georgia Tech and Dr. David Argento at the University of Washington. Dr. Cressler was very interested in deploying our technique in his high-speed RF and radiation effects lab and providing us with access to RF transceivers. Dr. Argento is willing to provide access to a Neutron beam at the University of Washington.

EXTERNAL FUNDING

Proposal Submissions

1. National Science Foundation (NSF), CAREER, July 2018 (Not Funded)
   Title: “CAREER: Fundamental Reliability Analysis of Si FinFETs and Nanowires through Ionizing Radiation Effects Spectroscopy”
   Amount: “$500,000”
2. Office of Naval Research (ONR), submitted Jan 2019 (Funded)
   Title: “RHBD Through IRES and Intelligent Control”
   Amount: “$199,771”
3. National Reconnaissance Office (NRO), Director's Innovation Initiative (DII), July 2019 (Under Review)
   Title: “In-Situ Radiation Detection Using Existing On-Board Spacecraft Hardware”
   Amount: $250,805

Contracts/Awards Received

1. Office of Naval Research (ONR), submitted Jan 2019 (Funded)
   Title: “RHBD Through IRES and Intelligent Control”
   Amount: “$199,771”

Sponsored Program Capacity Building Activities

1. NSF-REU Panel

WHAT’S NEXT FOR THIS RESEARCH?

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

This work will be folded into future funding submissions. Additionally, the developed IRES technique will be used to “tease-out” intentionally manipulated and/or inserted features used to improve wireless network security using RF-DNA fingerprints. Space systems are looking to deploy software defined radios (SDRs) due to their configurability; thus, this work will be leveraged to determine the impact/role radiation has on the RF-DNA fingerprints themselves. The goal is to determine the extent to which total ionizing dose (TID) and transient radiation effects negatively impact the RF-DNA fingerprint features and inhibit correct identification of the transmitter.

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

The work conducted under this award provided the preliminary results and understanding needed to submit a proposal to the FY 2020 National Reconnaissance Office’s (NRO) Director Innovation Initiative. This proposal presents a novel technique for determining radiation exposure using on-board systems without impacting Size, Weight, and Power – Cost (SWaP-C) constraints. This work has provided the foundational understanding need for intentional feature manipulation to improve radio device identification within contested environments. This understanding will be part of an NSF SaTC submission this September.

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?

The largest barrier is the teaching load being demanded of my department. Currently, our department is requiring all faculty to teach the same loads, only allowing a reduction if a course buyout from grant funding is awarded. This is prohibitive to additional growth, especially for those faculty engaged in research building. I am currently at capacity unless systematic changes take place.

FINANCIAL ACCOUNTING

The approximate remaining budget is $ 7,266.32. As the final ledger is still pending, the approximation is estimated based on travel and expected final month expenditures not appearing on ledger. The remaining balance is due almost entirely to an overestimate of the Fringe Rates. All other line items are near $0. We believe these rates could be better estimated in the future, as based on historical expenditure differences in faculty salary during the academic calendar versus summer. The allocated funds could have been better utilized with appropriate estimates.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

NAME, Lead PI: Dr. Soubantika Palchoudhury

Co-PI(s): Dr. Abdollah Arabshahi
Other Personnel: N/A

Project Title: Investigating the Flow of Nanodrugs Through Bio-Inspired Hydrogel Channels

Date Submitted: 07/31/2019

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

One of the major limitations for implementing new nanoparticle-based drugs as novel solutions to some of the biggest medical challenges of the day is the low translation rate from preclinical studies to the clinical stage. There is a need for a more reliable preclinical tool, which can predict the relevant behavior (e.g., flow regime and flow velocity) of new nanodrugs within the human body. In this project we constructed a combined experimental and computational strategy as a new preclinical model to assess the flow and deposition of nanodrugs in physiologically relevant environments. This project facilitated research training and support for graduate and undergraduate students. It has led to six publications, five external proposal submissions, four external conference presentations, and one undergraduate Honors thesis. Community engagement through outreach activities at local schools and UTC events for promoting science and technology fields was also supported through this grant. This work directly aligns with the SimCenter's mission to advance and support innovations in health and biomedical fields through cutting-edge interdisciplinary research.

INVESTIGATING THE FLOW OF NANODRUGS THROUGH BIO-INSPIRED HYDROGEL CHANNELS

Technology Area of Interest: HEALTH/BIOMEDICAL

PROPOSED TECHNICAL APPROACH

- Synthesis of novel bio-inspired flow paths for understanding the in vivo transport of nanodrugs
- Computational and experimental flow studies of the nanodrugs through the biomimetic flow channels

OUTCOMES

- Research training and support for two graduate and five undergraduate students.
- Six publications, four external conference presentations, and five proposal submissions.

RESULTS

Figure 1. Hydrogel channel fabricated. (a) Image showing the polyhydroxyethyl methacrylate (p-HEMA) hydrogel channel and (b) optical microscopy image of the p-HEMA hydrogel.

In this project, we first investigated the material properties of different hydrogel formulations to find the best suitable biomimetic polymer. p-HEMA hydrogels were successfully synthesized and chosen as the preferred material for fabricating novel biomimetic flow channels, based on these experiments (Figure 1). We investigated the flow of iron oxide nanodrug through these new soft

OTHER INFO

Budget and Schedule

Total Budget:	$100,000.00
Actual Used:	$99,061.92
Balance:	$ 938.08

Total period of performance is 12 months.

Task 1: Recruiting students and investigation of different hydrogel formulations for flow channels.

Task 2: Fabrication of p-HEMA hydrogel flow channels, conference presentation, and publication.

Task 3: Experimental flow studies of nanodrugs using the biomimetic hydrogel channels, publication, proposal submission, and conference presentation.

Task 3: In silico CFD simulation of the flow of nanodrugs through the hydrogel channels, report writing, proposal submission, and preparation of the manuscript summarizing the final results.

Deliverables

- Final report detailing results, financials, and future work
- 5 journal publications detailing results and future work and 1 book
- 4 external conference presentations and 5 internal conference presentations detailing the results
- 5 proposal submissions for external funding

channels, both experimentally and using CFD simulation. The final findings are currently being summarized for publication in the Beilstein journal of Nanotechnology.	• 2 user proposals with Sandia National Labs awarded **Organization Information** (SP): Civil and Chemical Engineering, University of Tennessee at Chattanooga, Chattanooga, TN 37403 Phone - 423-425-5455 Email – soubantika-palchoudhury@utc.edu (AA): SimCenter, University of Tennessee at Chattanooga, Chattanooga, TN 37403 Phone – 423-425-5485 Email – abi-arabshahi@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Nanoparticle-based drugs are seen as a solution for several current medical challenges as they can provide both diagnostic and therapeutic potential. One of the key challenges in translating a new nanodrug from invention to clinical application is the gap between the preclinical animal model studies to the clinical trials on humans. The goal of this project was to construct a new preclinical technique combining experimental and computational strategies for accurately predicting the flow of nanodrugs *in vivo*.

The scientific aims of this project were (i) Synthesis of hydrogel-based biomimetic channels for the experimental investigation of the flow of nanodrugs, (ii) constructing a new computational fluid dynamic (CFD) model to predict the flow of nanoparticle-based drugs over different flow regimes for paths replicating physiological environments of clinical relevance, and (iii) validation of the CFD model using the experimental flow studies of the nanodrug to construct a robust preclinical tool to assess new nanoparticle-based drugs.

We were able to successfully synthesize a p-HEMA-based hydrogel formulation as the biomimetic material for the flow channels. The flow channels were fabricated by pouring the hydrogels through plastic channels of targeted dimensions, followed by overnight solidification of the gels. The hydrogels were then removed from the plastic scaffolds to form the flow paths for the nanodrug. We used a new Pt-iron oxide nanodrug synthesized in the PI's laboratory for the flow studies. The experimental flow velocity and particle deposition were measured for eleven different concentrations of the nanodrug to understand the mechanism of flow. The CFD model to predict the flow of this nanodrug through the biomimetic hydrogel paths was constructed in parallel to these experiments using the Tenasi flow solver. The key accomplishments of this project are briefly summarized below:

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Recruitment of graduate and undergraduate students for the project	Two graduate and five undergraduate research students worked on this project. The students

	presented their results at both external and internal conferences.
Synthesis of the iron oxide nanoparticle-based drug	The nanodrug was successfully synthesized.
Synthesis of different hydrogels to find the best suitable biomimetic formulation	p-HEMA hydrogels were successfully synthesized using various literature reports.
Construction of flow channels for the nanodrugs with the hydrogels	The flow paths were fabricated for the first time using p-HEMA hydrogels.
Experimental flow studies of the nanodrugthrough the biomimetic flow paths	Experimental flow investigations were conducted through the hydrogel flow paths using eleven different concentrations of the iron oxide-based nanodrug.
CFD simulation to predict the flow of nanodrugs through the bio-inspired channels	The velocity and deposition of the nanodrugs over different flow regimes were modeled using Tenasi flow solver. The project has resulted in six publications. It has led to submission of five external proposals. The project has also supported four external and five internal conference presentations and one undergraduate Honors thesis.
Validation of the computational model using the experimental results	The final findings of this project are currently being summarized in a journal article to be submitted at the Beilstein journal of Nanotechnology.

Challenges & Strategies Used to Address / Overcome: .

Most of the computational models used for studying the transport of nanodrugs to date showed limited experimental validation. Therefore, one of our challenges was to choose appropriate design parameters for the CFD model that will be clinically relevant. It was also challenging to design the flow experiments, primarily due to the novelty of this project. Each of these challenges were overcome via extensive literature search, research discussions between the PIs, as well as discussions at professional meetings and conferences.

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

One area of further research will be to measure the actual roughness of the hydrogel flow channels for further enhancing the CFD flow model for the nanodrugs. Incorporating the accurate material properties of the flow paths (e.g., roughness factor) in the model will lead to a more reliable prediction of the flow of nanoparticles. One way to further investigate the roughness of the flow channels will be through analysis of electron microscopy images of the hydrogels.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This project facilitated successful recruitment of graduate students and laboratory start-up for the PI. The PI was able to start a new research direction of understanding the transport and interaction of nanoscale drugs during drug delivery through a combination of experimental and computational approach. This project led to submission of external grants for the PI and the co-PI. It has also facilitated key research collaborations with Sandia National Laboratory and the University of Buffalo. The project has resulted in several collaborative publications and conference presentations for both PIs.

Students Impacted .

1. Eric Pritchard, 1st year M.S. Chemical Engineering candidate – Full tuition, graduate assistantship, and health insurance of the student was supported from the grant. The student was mentored in CFD modeling and was involved in constructing the computational flow model for the nanodrugs.
2. Armel Boutchuen, 2nd year M.S. Chemical Engineering candidate – The student was involved in synthesis and characterization of the nanodrug and the hydrogel channels, flow studies of the nanodrug through the hydrogel channels, writing the journal article, and presenting the results at conferences.
3. Ketan Patel, Chemical Engineering undergraduate student, graduated in May 2019 – Hourly support for the student was provided through this grant. The student was involved in synthesis and material characterization of the hydrogel channels, writing the journal article, and conference presentations.
4. Olivia George, Chemical Engineering undergraduate student, graduated in May 2019 – The student was involved in cutting-edge experimental research related to this project and conference presentations. She won the NSF Graduate Student Fellowship and completed the Honors Thesis under the PI's supervision.
5. Yasmin Foster, Chemical Engineering undergraduate student, graduated in May 2019 – She was involved in hydrogel synthesis and flow experiments as well as helping with the journal article.
6. Dell Zimmerman, Chemical Engineering undergraduate student, junior – The student was extensively involved in the experimental section of the project, presenting at different internal conferences, report writing, and outreach activities at local schools to promote science, technology, engineering, and mathematics. Won the best poster award at the UTC Technology Symposium.
7. Gitapun Jur, Chemical Engineering undergraduate student, sophomore – Involved in experimental research related to the project and presentation at internal conferences.

Community and Broader Impacts

This project addresses one of the key scientific challenges in the application of next-generation nanodrugs at the clinical phase – limited knowledge of the flow and behavior of nanodrugs inside the human body as opposed to the animal model studies at the preclinical stages. The novelty of this research is the use of a new computational model in combination with flow experiments through newly synthesized biomimetic channels to understand the flow of

nanodrugs in a physiologically relevant environment. This work will have immense significance in drug delivery and biomedical applications in terms of designing a first-of-its-kind preclinical model to accurately assess nanoscale drugs in physiologically relevant conditions. The project has led to research training and professional development through conference presentations for two graduate and five undergraduate students. The PIs have conducted science experiments at two local schools and two community events organized by UTC to promote science, technology, engineering, and mathematics (STEM) among the school students. The PIs have also organized events in collaboration with the UTC Society of Women Engineers (SWE) student chapter to enhance participation of female students in STEM fields.

Scholarly Products

Publications:

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

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

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

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

Palchoudhury, **S**., Jungjohann**, K., Weerasena**, **L**., **Arabshahi**, **A**., Gharge, U., Albattah, A., Miller, J., Patel, K., Holler, R., "Enhanced legume root growth with pre-soaking in α-Fe_2O_3 nanoparticle fertilizer." *RSC Adv*, 2018. 8:p. 24075. Impact Factor: 3.049

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

External Conferences:

Palchoudhury, S.; **Arabshahi**, **A**.; Gharge, U.; Boutchuen, A. Foster, Y. Zimmerman, D. Alresheedi, H. "A new class of integrated chalcogenide nanocrystals and thin films for solar cell applications" 2019 TMS Conference, Mar 2019 (Oral Talk).

Palchoudhury, **S**., **Arabshahi**, **A**., Foster, Y., Gharge, U., Boutchuen, A. "Synthesis and size analysis of DNA conjugated bio-hybrid nanostructures" Materials Research Society Fall Conference, Nov 2018 (Poster).

George, O., **Palchoudhury, S**. "Effect of different ligands on water-soluble iron oxide nanoparticle size" AIChE Conference, Oct 2018 (Poster).

George, O., Mcmahon, W., **Arabshahi**, **A**., **Palchoudhury**, **S**. "Synthesis and transport of Pt-iron oxide nanodrugs" National Council of Undergraduate Research Conference, Apr 2018.

Presentations at UTC:

Palchoudhury, S. “A materials perspective of oil spill remediation and plant interactions with nanoparticles,” The Inaugural Workshop of Southeastern Computational and Geospatial Environmental Hydrology organized by UTC SimCenter and Geology, Feb 2019 (Oral Talk)

George, O., Zimmerman, D., Foster, Y., Patel, K., Jur, G., **Palchoudhury**, **S**. “Effect of different ligands on water-soluble iron oxide nanoparticle size” Technology Symposium, Apr 2019 (Poster)

Boutchuen, A., **Arabshahi**, **A**., **Palchoudhury, S**. “Synthesis and size analysis of bio-hybrid nanostructures” Technology Symposium, Apr 2019 (Poster)

George, O. “Synthesizing multifunctional iron oxide nanodrugs and developing a model for their size analysis using dynamic light scattering” Research Dialogues, Apr 2019 (Oral Talk)

Zimmerman, D., Boutchuen, A. “Characterization and biological response of legumes fertilized with engineered nanoparticles” Research Dialogues, Apr 2019 (Oral Talk)

Inventions or Other Intellectual Property

None

Research Outreach & Collaboration

This project has helped establish external research collaborations with eminent scientists from Sandia National Laboratories, University at Buffalo, and The University of Alabama who are working in the field of biomedical nanotechnology and drug delivery. The PIs will continue to maintain these research collaborations. A few key collaborators are:

- Dr. Katherine Jungjohann, Center for Integrated Nanotechnologies, Sandia National Laboratory
- Dr. Sergei Ivanov, Center for Integrated Nanotechnologies, Sandia National Laboratory
- Prof. Arunava Gupta, Chemistry, Chemical and Biological Engineering, and MINT Center, The University of Alabama
- Dr. Karthik Ramasamy, UniQD Inc., New Mexico
- Dr. Nirupam Aich, Civil, Structural and Environmental Engineering, University at Buffalo

EXTERNAL FUNDING

Proposal Submissions

1. “A New Library of Cadmium-Free Multinary Chalcogenide Nanocrystals for Engineered Quantum Dot Light Emitting Device”, PI: S. Palchoudhury, $508,356, NSF Career, Engineering Directorate, Division of Electrical, Communications and Cyber Systems, submitted: July 2019
2. “Evaluation of an Integrated Nanophotocatalytic and Bioremediation Approach to Stormwater Management using Rain Barrels as a Green Infrastructure”, PI: S. Palchoudhury, co-PI: M. Danquah, $199,891, Tennessee Department of Transportation, submitted: April 2019
3. “A New Class of Enhanced Sensors with Iron Oxide-Protein Cage Nano-architectures for Petroleum Tracers”, PI: S. Palchoudhury, $55,000, ACS Petroleum Fund, submitted: March 2019

4. “Characterization of a new class of integrated copper chalcogenide nanocrystals”, PI: S. Palchoudhury, User research proposal for Center for Nanophase Materials Sciences, Oak Ridge National Laboratories, submitted: March 2019
5. “Coupled Computational and Experimental Approach to Understand the Flow of Nanodrugs”, PI: S. Palchoudhury, co-PI: A. Arabshahi, $300,763, NSF Engineering Directorate, Division of Chemical, Bioengineering, Environmental and Transport Systems, submitted: January 2019

Contracts/Awards Received

1. Center for Integrated Nanotechnologies User Proposal Award, Sandia National Lab, “Understanding the Effect of Engineered Nanoparticles in Agriculture”, 2017-2018, PI: S. Palchoudhury, Agreement for electron microscopy use
2. Center for Integrated Nanotechnologies User Proposal Award, Sandia National Lab, “Developing a New Family of Wurtzite $CuZn_2ASe_4$ (A= Al, Ga, In) Nanocrystals for Solar Cell Applications”, PI: S. Palchoudhury, Agreement for electron microscopy use
3. NSF REU-site: “Engaging Undergraduates in Interdisciplinary Computing in Biology (ICompBio)”, PI: H. Qin, co-PI: S. Palchoudhury, 2019-2022, $359,484
4. UTC Faculty Development Grant 2019 for summer research, “Experimental and numerical simulation of nanoparticle flow through hydrogel channels”, PI: S. Palchoudhury, co-PI: A. Arabshahi, $1,500. (Internal Funding)

Sponsored Program Capacity Building Activities

1. Attended NSF 2019 Biology REU Site Workshop, April 4–6 2019, Arlington, VA.
2. Attended on-campus NSF Career workshop activities.

WHAT’S NEXT FOR THIS RESEARCH?

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

I will continue to engineer hydrogel and 3D bio-printing based biomimetic structures to represent physiologically relevant systems for drug delivery. I will also continue to investigate the flow of different nanodrugs through these channels to establish a robust preclinical model that can facilitate a significantly higher success rate for new nanodrugs at the clinical phase.

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

Synthesis of new materials and device fabrication for next-generation flexible and wearable biomedical devices is one of the primary research areas I will pursue.

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?

We are seeking external funding to support the computational time and the expensive experimental work required for the next phase of the project.

FINANCIAL ACCOUNTING

N/A

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Hong Qin, Lead PI

Co-PI(s): Joey Shaw, Yu Liang, Craig Tanis

Project Title: Analyzing Bioimage Big Data With Deep Learning Neural Networks

Date Submitted: 03/05/2018

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

We developed various machine learning methods, including deep learning methods, to extrapolate meaningful biological information or meta-information from bioimage data sets. For the yeast time-lapse microscopic images, we compared convolutional neural networks with capsule networks, and found that the two methods have complementary performances. For the plant image data sets, we experimented with various architectures of convolutional networks to compare flowering versus non-flowering images and extract the color pixel panel for color correction.

Analyzing bioimage big data with deep learning neural networks.

Technology Area of Interest: Health and Biosystems

PROPOSED TECHNICAL APPROACH

- *Objective 1: Develop convolutional neural networks (CNNs) to predict cell division events from microscopic images of dividing yeast cells.*
- *Objective 2: Develop convolutional neural networks to significantly improve current prediction accuracy using herbarium sheets.*

OUTCOMES

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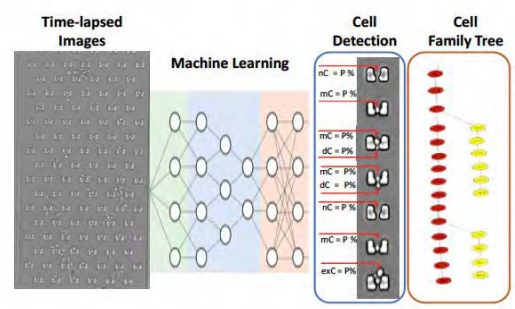
1. For the yeast time-lapse microscopic images, we compared convolutional neural networks with capsule networks, and found that the two methods have complementary performances. We also prototype a RCNN method to detect cell objects and subsequent lifespan inferences.
2. For the plant image data sets, we experimented various architectures of convolutional networks to compare flowering versus non-flowering images and extract the color pixel panel for color correction.
3. *We have 2 accepted journal publications, 1 extended conference abstract, several conference presentations, 1 funded NSF grant, 1 pending NSF grant, and 1 NIH grant submission.*

RESULTS

1. 

We prototyped a RCNN method to detect cell objects, and a maximal likelihood method to generate cellular family tree, and lifespan inference.
2. We compared CNN and Capsule networks using our microscopic images, and found they have complementary performance.
3. We prototyped a Fast RCNN software for color chip detection. This method is being integrated into an automated pipeline for herbarium sheet processing.

OTHER INFO

Budget and Schedule

Total Budget:	$99,957.00
Actual Used:	$91,445.70
Balance:	$ 8,501.30

Total period of performance is 12 months.

Task 1: Months 1-12

Task 2: Months 1-12

Deliverables

- Final report detailing results, financials, and future work
- Publication
- External and internal conference presentations
- External grants applications

Organization Information

Hong Qin

423–425–4329, hong-qin@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Objective 1: Develop convolutional neural networks (CNNs) to predict cell division events from microscopic images of dividing yeast cells.	We prototyped a method that can evaluate cell divisions from time-lapsed images. Initially, microscopic time-lapsed images are converted to sub-images for individual traps. These sub-images were labeled and used to train a machine learning method to identify cells features such as coordinate, area, confidence rate, class, etc. A null distribution of cell movement was generated to evaluate cell movements. We then developed a maximum-likelihood algorithm for cell tracking between images at different time-points and inferred a cell family trees through a trace-back method. Finally, the branching patterns of the cell family tree were used to infer replicative lifespan of yeast. The proposed method is an automatic machine learning-based prototype using a Maximum Likelihood Algorithm (MLA) and a Bayesian approach to infer yeast replicative lifespan measurements from time-lapsed images. This generic method has the potential to not only accelerate the efficiency but also expand the range of quantitative measurement of yeast replicative aging experiments. We compared the image classification performance of CapsuleNet and Convolutional Neural Networks using our microscopic images for dividing cells. We found that CapsuleNet and CNN have complementary performance. A combination of these two models yields the best performance.
Objective 2: Develop convolutional neural networks to significantly improve current prediction accuracy using herbarium sheets.	The digitization of natural history records, such as herbarium specimens, is generating a large dataset with many unexplored novel applications. Despite this growth, the workflow for digitizing herbarium sheets is very labor intensive, with very few applications written to improve or automate this. Using a domain-specific neural network, we are able to automate the correction of some post-processing workflows, such as automatic color correction and white balance, and improve the performance of selective search and current state-of-the-art neural networks

Challenges & Strategies Used to Address / Overcome:

Generating high-quality training images was a challenge that we experienced. We were able to address this problem through image augmentation.

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

We were surprised that CapsuleNet did not outperform CNNs architecture for the image classification of dividing cells. Although this finding most likely is not the final saying on the performance of CapsuleNet, our results certainly suggest that CapsuleNet may not be a superior solution for bioimage classification, and significant improvement may be needed.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

PI Qin's effort in this project is synergistic with his effort on NSF Big Data Spoke project. The collaboration of this project led to one NSF CUE proposal application and one NIH R21 grant application. PI Qin mentored the graduate students, postdoc researcher, and undergraduate researchers.

CoPI Yu Liang helped mentor the MS thesis of Mr. Justin Clark and mentored undergraduate researchers.

CoPI Tanis helped mentor the MS thesis of Mr. Justin Clark.

Students Impacted

Mehran Ghafari: A PhD student whose stipend and tuition was supported by this grant from July 2018 to June 2019. He led the task on Fast-RCNN for microscopic image analysis, and the comparison of CNN and CapsuleNet.
Justin Clark: MS graduate student. He performed the initial comparison of CNN and CapsulNet.

Caleb Powell: MS graduate student. He is the connection between computer science students and biology students. He led the development of herbarium automation pipeline.

Dakila Ledesma: Undergraduate researcher. He led the color chip task.

William Baker: Undergraduate researcher. He participated in plant image CNN task.

Andrew Watson: Undergraduate researcher. He participated in developing Python code for image partitions.
Haobo Guo: June salary was supported for Dr. Guo to help Mr. Ghafari to revise manuscript, including revise algorithms, figures, methods and materials, results and discussions.

Community and Broader Impacts

Undergraduate researchers in this project experienced an authentic research project. One of the students was accepted into the iCompBio NSF REU project during the summer of 2019 and is planning to apply for NSF Graduate Research Fellowship.

Scholarly Products.

Publications:

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

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

External Conferences:

Powell, C. Oral presentation. "Born Digital, enabling a field-database workflow for herbaria." 34th Annual Meeting of the Society for the Preservation of Natural History Collections. Field Museum, Chicago. May 25–30, 2019.

Powell, C. Oral presentation. "Born digital, addressing the challenges of a field-to-database workflow for collections based research." 80th Annual meeting of the Association of the Southeastern Biologists (ASB). Memphis. April 3–6, 2019.

Ledesma, Oral presentation, "Using convolutional neural networks to classify the reproductive state of digitized herbarium specimens." 80th Annual meeting of the Association of the Southeastern Biologists (ASB). Memphis. April 3–6, 2019.

Ghafari, Poster presentation, UAB

Ghafari, Poster presentation, Memphis.

Guo, H. Poster presentation, UAB.

Ghafari, Poster presentation, Finding inner modeler

Guo, H. Poster presentation, Finding inner modeler.

Guo, H, UTK 21st Century Cures meeting.

Ghafari, UTC 21st Century Cures meeting.

Presentations at UTC:

Ghafari, 3 minute elevator competition

Ghafari, poster presentation. UTC Research Day, Technical symposium.

Dax, Technique symposium.

Clark, Justin, Technique symposium.

Guo, H. UTC Research Day.

Guo, H. Technique symposium.

Inventions or Other Intellectual Property

Not Applicable.

Research Outreach & Collaboration

Dr. Weiwe Dang, Baylor College of Medicine, continued collaboration.

Dr. Zhaozheng Yin, SUNY Stony Brooks, continued collaboration.

Dr. Eming Guven, continued collaboration.

EXTERNAL FUNDING

Proposal Submissions

1. Qin (PI), Dumas, Shaw, NSF CUE: Collaborative Research: Bridging diversity and curriculum gaps in computing through pedagogical innovation and cross-discipline education. $114K. Submitted on May 9, 2019.

2. Qin (Senior personnel), NSF Data Science Corps, Collaborative Research: Building Diverse Workforce in Data Science Through Integrating Real-world Projects into Curricula. ~$360K. PI Yang. Submitted in February 2019.

3. Qin (PI), NIH R21, Using permutation of gene/protein networks for pairwise association analysis of genomic data. ~$300K, Submitted on Nov 16, 2018.

4. Liang (PI), Dalei Wu (Computer Science & Engineering), Cuilan Gao (Mathematics), Hemant Jain (Management), and Dr. Anthony Skjellum (SimCenter) have requested $723,641 from the National Science Foundation for the project entitled, “HDR DSC: Collaborative Research: ADACE – Anthropocentric Data Analytics for Community Enrichment.” Submitted in February 2019.

Contracts/Awards Received

1. Qin (PI), Liang (coPI), Shaw (coPI), Hossain (coPI), NSF IIS, “Spokes: MEDIUM: SOUTH: Collaborative: Integrating Biological Big Data Research into Student Training and Education”, $1M, ~$550K to UTC, Oct. 2018 – Sep. 2021, awarded.
2. Qin (PI), Palchoudhury (coPI), NSF DBI “REU Site: ICompBio – Engaging Undergraduates in Interdisciplinary Computing for Biological Research” ~ $359K. Submitted in August 2018, awarded.

Sponsored Program Capacity Building Activities

1. PI Qin led postdoc Haobo Guo and graduate student Mehran Ghafari attended the NIH 21st Century Cures Conference at UTK in March 2019.
2. PI Qin led postdoc Haobo Guo and graduate student Mehran Ghafari attended the NSF workshop, Finding Your Inner Modeler at UAB in June 2019.

WHAT’S NEXT FOR THIS RESEARCH?

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

Qin plans to submit 1 NSF proposal, and 1 NIH proposal in the immediate future.

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

PI Qin has on-going research interests in biological big data, image analysis, machine learning, algorithm development, network analysis and modeling

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

Not applicable.

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

Not applicable.

FINANCIAL ACCOUNTING

Residual funding occurred because UTC accounting considered June 2018 summer support of PI Qin as additional pay in the budget year of 2018–2019, which prevented further effort of PI Qin in the project.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Mina Sartipi, Lead PI

Co-PI(s): Nancy Fell
Other Personnel: N/A

Project Title: Improving Post-stroke Management Efficiency and Patient Outcomes through Analytics

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

For the main task of the CEACSE project (TN Higher Education Commission), we primarily focus on developing a data-driven precision healthcare ecosystem for management for stroke. The goal of this task is to utilize machine learning/deep learning framework for data processing, modeling, and decision support in healthcare management. The development of predictive models for stroke management will allow us to help health outcomes and increase stroke patients' quality of life by providing a sophisticated and detailed analysis of post-stroke assessment. Furthermore, it will help reduce the cost of stroke management, and reduce caregiver's burden.

In order to achieve this goal, we use the medical data provided by the TN Department of Health (TDoH) and the Centers for Medicare and Medicaid Services (CMS), which includes patient demographic information, and clinical information such as primary diagnosis codes (ICD9), procedure codes, source of admission, and insurance status. We propose a machine learning/deep learning-based methods (Logistic Regression, Random Forest, AdaBoost, and Multi-layer Perceptron) to extract patient information and discover underlying patterns from the data. All of the methods mentioned above were implemented using scikit-learn and Keras, a deep learning library written in Python.

Using the simplest model (i.e., logistic regression model), we were able to build an easy-to-use predictive tool for predicting hospital discharge disposition status of stroke patients.

A general overview of the end-to-end post-stroke predictive analysis system is shown in figure 1. Based on this architecture, we were able to calculate the risk scores associated with the probability of facility discharge. Figure 2 shows the receiver operating characteristic (ROC) curves and the corresponding are under the curve (AUC) estimates for different models predicting hospital discharge disposition status of stroke patients (home discharge vs. facility discharge).

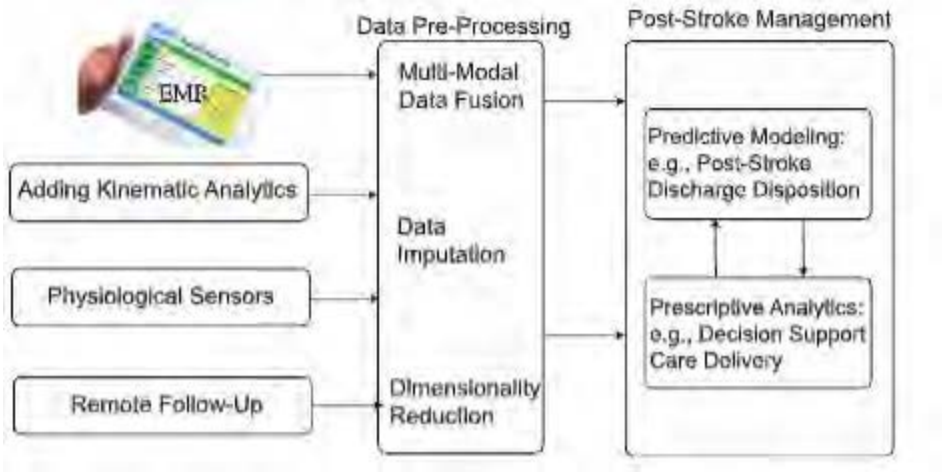


Figure 1. End-to-end post-stroke predictive analysis system

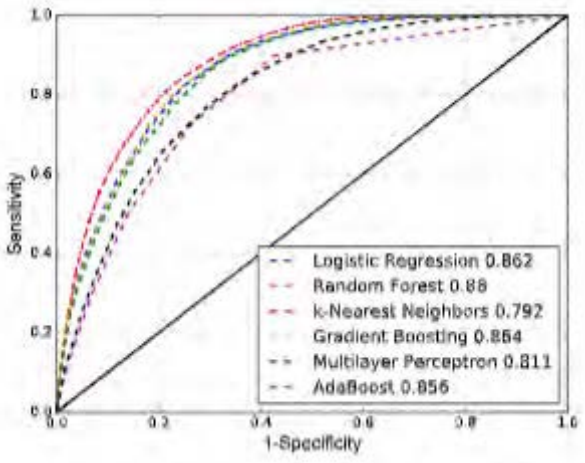


Figure 2. The result of early prediction of hospital discharge disposition status

PROJECT TITLE

Improving Post-stroke Management Efficiency and Patient Outcomes through Analytics

PROPOSED TECHNICAL APPROACH	OUTCOMES
• Utilizing machine learning / deep learning methods to pre-process medical data and build a predictive model. Also, we addressed the issues of feature scoring mechanism in machine learning models. Finally, an easy-to-use clinical predictive tool was developed to assist clinicians in making decisions about their patients.	• J. Cho, A. Alharin, Z. Hu, N. Fell, and M. Sartipi, "Predicting Post-stroke Hospital Discharge Disposition Using Interpretable Machine Learning Approach". Submitted to IEEE Big Data Conference 2019
RESULTS	**OTHER INFO**
	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

Table1. Total risk score calculation

Beneficiary ID	Discharge Status	Gender	Age	Stroke Type	...	Total Risk Score
A	1	1	3	5	...	11
B	0	0	3	1	...	4
C	1	0	1	0	...	2

Table2. Total risk score conversion

Beneficiary ID	Total Risk Score	Actual Discharge Status (y)	(Threshold = 9) Predicted Discharge Status ($\hat{y}$)
A	10	facility	facility
B	7	facility	home
C	14	facility	facility
D	4	home	home
E	9	facility	facility

Figure 2. Predicted and observed probabilities of facility discharge for each total risk score.

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Integrating an end-to-end ML/deep learning framework for data pre-processing, predictive modeling, and data-driven decision support in healthcare management	• ML/DL methods were used to pre-process data, reduce the dimension of data, and for predictive modeling. An end-to-end ML/DL framework was developed based on the aforementioned processes to have a system that could process data and provide significant clinical decisions.
Solving unaddressed issues of deep learning on feature ranking/feature importance scoring	• Utilized LIME (Local Interpretable Model-Agnostic Explanations Model) to analyze black-box models (ML/DL) to see what is going on within the model and to find which features are more important.
Designing predictive models for health outcomes considering quality of life and caregiver burden	• In our predictive model, we have considered patient's demographic and clinical information to build a model around the patient (patient-centric), and the analysis was done in acute admission rather than post-discharge situations. This was done to help clinicians and caregivers to obtain information early on to prepare for post-stroke management.
Building easy-to-use clinical predictive tools based on feature importance scores of raw input data.	• Using the simplest model (logistic regression), we were able to obtain coefficients from performing multivariate logistic regression. The coefficients from the regression were converted into a single digit integer that is used to represent the probability of facility discharge.

Challenges & Strategies Used to Address / Overcome:

There were several limitations to the study. The findings are limited to only a few years of hospital data and may not be generalizable to all patients post-stroke. Some patients may have lost insurance coverage after discharge. Risk scores were calculated based on index hospitalization for stroke; however, we could not know if this was the patient's first stroke or if it was a recurrent stroke with the first stroke occurring prior to our dataset. Patients with recurrent strokes would likely be considered at higher risk for facility discharge, however, this could not be accounted for without a full admission history. When validating the predictive tool via

readmission analysis, the threshold to determine when the algorithm would predict facility versus home discharge was arbitrarily set at 75% probability of facility discharge. However, this threshold could likely be adjusted to allow for a closer match between predicted and actual discharge dispositions. Collaborating with hospital administrators or physicians may allude to a more clinically meaningful threshold that increases confidence in relying on the predictive tool.

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

We originally used patient's source of admission as one of the variables in predicting their discharge disposition status; however, it is difficult to determine whether the disparity in outcomes is due to the patients' medical complexity or the type, quality, and amount of care received at a skilled nursing facility. Because of this, admission source may not be an insightful variable that adds to general clinical reasoning. Eliminating this variable may depress the risk scores and give greater weight toward comorbidities and stroke type.

Additionally, details of each patient's characteristics are limited to the amount of detail in their claim. We did not track the role of factors such as functional status, treatment received during the acute care stay, or patient and family preference in determining discharge status. These factors may provide deeper insight into a patient's profile. Lastly, while readmission rates is a well-accepted measure of quality of care, we are unable to distinguish if any given readmission was due to inappropriate discharge planning or poor quality of care along the patient's journey.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This research required significant interprofessional collaboration between computer science and physical therapy students and professionals. As such, a tremendous amount of time was spent by all engaged in the research to learn about the others' professions, their terminology and standards of practice.

Students Impacted

Jin Cho, PhD student in the Computer Science and Engineering Department

Kristal Price, Physical Therapy Department

Rebecca Salstrand, Physical Therapy Department

Community and Broader Impacts

Scholarly Products

Publications:

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

Presentations at UTC:

1. **M**. **Sartipi**, UTC Research Dialogues

Inventions or Other Intellectual Property

None

Research Outreach & Collaboration

EXTERNAL FUNDING

Proposal Submissions

We are working on a proposal to be submitted to NIH or NSF SCH.

Contracts/Awards Received

N/A

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?

N/A

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

N/A

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

N/A

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

NAME, Lead PI: Kidambi Sreenivas, PhD

Co-PI(s): Abi Arabshahi, PhD, Ethan Hereth, PhD
Other Personnel: N/A

Project Title: Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities

Date Submitted: 02/27/2017

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

The objective of this project was to reconstitute the capability at the SimCenter in order to carry out city-scale simulations. The first step in this process was the development of an efficient workflow that could be used to process the Geographical Information Systems (GIS) data into usable geometry. Once this process is completed, meshes can be generated and simulations carried out.

The biggest challenge when it comes to any simulation is that of geometry. Having a clean, high-quality geometry results in a good quality mesh, which in turn enables the simulation to complete successfully. The building footprints of various cities are available through their respective GIS departments. This data is in the form of ShapeFiles and needs to be manipulated and exported into a format that is conducive to building a mesh. This was carried out using a combination of ArcGIS (commercial GIS software), various libraries in Python, and some custom code. This workflow enabled the efficient processing of GIS information into a water-tight solid model that was then used within Pointwise (commercial grid generation software) in order to generate the final mesh.

This project provided three undergraduate students with research experience in utilizing ArcGIS, Python, and Pointwise. This resulted in two of the students obtaining summer internships at NASA Ames Research Center. The third student obtained a year-long internship with an industrial boiler design and installation company in the Dalton area. Additionally, this project resulted in research collaborations between various faculty at UTC and produced five related proposals.

Urban Resilience in the Post-Evacuation Age: Combining CFD and ABM for Megacities

Technology Area of Interest: Energy and the Environment

PROPOSED TECHNICAL APPROACH

Utilize available GIS data in order to model airflow through an urban area:

Task 1: Process GIS data in ArcGIS

- Obtain GIS data (building footprints and height data) for New York City (NYC)
- Simplify GIS data by combining buildings in close proximity
- Export Shapefiles

Task 2: Generate building geometry

- Process shapefiles in Python to eliminate courtyards and other features
- Export updated building footprints
- Use custom code to "raise" buildings to appropriate height and export solid model

Task 3: Generate mesh

- Generate mesh using Pointwise

Task 4: Carry out simulations and agent-based modeling

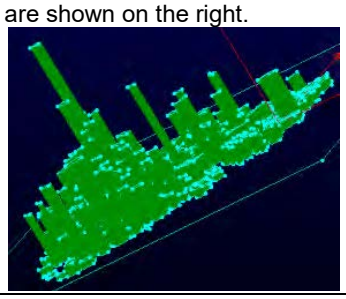
- Run simulations
- Share results to enable agent-based modeling

OUTCOMES

The toolchain required to carry out simulations of airflow through urban areas has been reconstituted. It required the use of a combination of ArcGIS, Python, custom code, and Pointwise in order to achieve the desired objectives. This process also exposed undergraduate students to research areas that resulted in them obtaining summer internships at NASA Ames. Additionally, this project has enabled the submission of five proposals (NSF, TDOT, USGS, and the Lyndhurst foundation). Additional areas of collaboration for agent-based modeling involving UTC faculty have been identified and will be pursued in the near future. A presentation regarding the status of the project was given at UTC Research Dialogues and further publications of the results in peer-reviewed journals will be pursued.

RESULTS

The two figures above illustrate the process in ArcGIS wherein some of the finer features (like courtyards) were agglomerated into the building footprints. This reduced the complexity of the overall geometry. The resulting footprints were further processed using Python and resulted in the representation of the footprints (image on the left). These footprints were then converted into buildings and the results are shown on the right.



OTHER INFO

Budget and Schedule

Total Budget:	$77,464.00
Actual Used:	$65,526.68
Balance:	$ 11,937.12

Total period of performance is 12 months.

Task 1: Months 1-6
Task 2: Months 3-9
Task 3: Months 6-12
Task 4: Months 9-12

Deliverables

- Efficient workflow to go from GIS data to flow simulations.
- Final report detailing results, financials, and future work
- Publications, if any
- External and internal conference presentations

Organization Information

Department of Mechanical Engineering, 615

Meshes were generated using the solid model generated above and simulations are being carried out. These will be provided to researchers at NYU as inputs to the agent based models. Additional agent-based modeling will also be carried out at UTC.	McCallie Avenue, Dept. 2074, Chattanooga, TN 37403

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The figure shows a 3D model of a section of New York City (Manhattan) downloaded from http://nyc.gov. This looks precisely like something that would be needed in order to be able to simulate the airflow through NYC. While the model looks visually realistic and can be used for visualization purposes, it is not appropriate for simulations. The main reason for the inappropriateness is that the model is not watertight. The practical consequence of this limitation is that a volume mesh, the necessary first step before a simulation, cannot be generated using this geometry. Furthermore, cleaning up this geometry so that the model becomes watertight is very labor intensive as each building has to be checked individually. Additionally, there are many buildings which are not very tall (and hence do not affect the airflow significantly) that are included in this model. Including these buildings in the simulations increases the number of mesh points that are required, thereby increasing the resource requirements. In order to alleviate some of these issues, a different approach was taken.

NYC also provides coordinates of building footprints in addition to heights of the buildings themselves. This data can be used to “raise” the buildings from the ground up. Such a process ensures that the resulting geometry is watertight. Additionally, this process of utilizing the footprints and heights allows for some simplifications of the baseline geometry. NYC has a very high building density and this can be used to replace a number of closely spaced buildings with a single large building by agglomerating the footprints and averaging the heights of the buildings. Furthermore, building below a certain height threshold or below a certain square-footage can be eliminated. An example of this approach is shown in the figure below wherein certain geometric features have been agglomerated in the figure on the right (highlighted area).

Once these manipulations have been carried out, the resulting footprints are raised to the appropriate heights resulting in a watertight geometry. This geometry is then imported into Pointwise in order to generate a volume mesh that can be used for simulations. The table below highlights the steps involved in the overall process.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Task 1: Process GIS data in ArcGIS	This task was successfully accomplished, though there is room for improvement. ArcGIS has a number of features that can be explored in order to improve the quality of the resulting shapefiles.
Task 2: Generate Building Geometry	This task depends on the output from Task 1 and was accomplished using a combination of Python libraries and custom code. Several features were added to the custom code and various options in the Python libraries were used to improve the output.
Task 3: Generate Mesh	This task requires the output from Task 2 to be of good quality. The resulting geometry was processed using Pointwise in order to obtain a valid and good quality mesh.
Task 4: Carry out simulations and agent-based modeling	This task is still ongoing and will be completed in the next couple of months. The slippage in the schedule was a result of a lack of time on part of the PIs which delayed the processing of the GIS data.

Challenges & Strategies Used to Address / Overcome:

There were two significant challenges associated with this project: (1) High building density in NYC*:* While the PIs had worked with GIS data from Washington DC and Chattanooga in the past, the sheer number of buildings in Lower Manhattan posed a unique challenge. Furthermore, the density of the buildings was very high, the consequence of which was that the "gaps" between buildings were very small compared to their overall dimensions. This required significant manipulation of the GIS data so that buildings in close proximity were "merged" into a single structure. In order to successfully accomplish this and avoid agglomeration across roads and highways, constraints in terms of street locations had to be imposed. Additionally, options in ArcGIS were utilized to ensure that building footprints were "square" which helped improve the overall quality of the consolidated footprints. (2) Significant constraints on time on part of the PIs: The PIs on this project were involved in multiple sponsored projects in addition to their regular teaching and system administration responsibilities. This put a significant constraint on

the amount of time the PIs could dedicate to the project. An undergraduate student, who was familiar with ArcGIS was utilized to process the GIS data. This helped alleviate some of the time constraints faced by the PIs. However, that was not sufficient to overcome the schedule slippage. The end result is that the workflow required to go from GIS data to a valid mesh has been established and simulations are underway and are expected to be finished in the next couple of months.

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

The main area where we did not meet our goals was having a successful simulation of air flow through NYC and interface the same with the agent-based code in order to carry out virtual evacuations. However, the ground work to achieve this efficiently has been laid and the next time we're faced with an urban simulation scenario, we should be able to finish it in the desired time period. This was a consequence of both the high building density and the time constraints faced by the PIs.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This project has spawned new collaborations between the PI and Dr. Spratt (Biology). It is anticipated that this new collaboration will result in proposals and publications. This should positively impact the carrier of the PI.

Students Impacted

Juan Hernandez: Juan was an undergraduate student who was working for the PIs when the project started. His experience with Pointwise (honed through this project) came in handy for his Honors thesis which required him to generate meshes for nozzle geometries. Juan graduated with a BS in Mechanical Engineering in Spring 2019 and currently has a year-long internship with National Boiler Service, an industrial boiler design and refurbishment company based out of Dalton, GA.

Hannah Gifford: Hannah was also an undergraduate student who was working for the PIs when the project started. She graduated in Spring 2019 with a BS in Mechanical Engineering and a minor in Computer Science. Her background made her uniquely suited for this project and the experience with Pointwise and Python helped her earn a summer internship with the Helios group (helicopter simulation software) at NASA Ames Research Center. She may consider going to graduate school, but at this time, her plans are to obtain a job in industry.

Aaron Crawford: Aaron was a junior when the project started and had some background with ArcGIS when he started. He was utilized to process the building footprints. Additionally, he learnt Pointwise and Python through this project. This combination helped him earn an internship with the Helios group at NASA Ames Research Center. He will be returning in Fall to complete his senior year and is on track to graduate in Spring 2020. He will also be utilizing the skills he has developed through this project and his internship in order to finish his Honors thesis. He is hoping to pursue graduate studies once he has graduated with the BS in Mechanical Engineering.

Community and Broader Impacts

The research carried out as part of this project resulted in an efficient workflow that can be used to model flow through urban areas. This technology is not restricted to densely populated areas; it can be applied to various other scenarios such as communicable disease transmission, flow inside aircraft cabins, etc. These applications can have tremendous societal impact as Ebola, influenza, and other communicable diseases are emerging as potential global threats.

Additionally, the agent based modeling can be applied in a variety of scenarios. For example, agents can be created who represent, for example, citizens of Chattanooga. These agents can then be used in simulations to see how they would react to a new piece of technology (for example autonomous vehicles) or proposed construction. This can be done in a virtual setting, thereby minimizing the risk of rejection.

The technology developed here can be applied to model airflow in an ICU to see if repositioning of the HVAC ducts from their standard location can result in improved outcomes for the patients by reducing the presence of bacteria on the surfaces near the patient. This can have a significant societal impact as the patients in ICUs are very vulnerable to such infections.

Scholarly Products

Publications:

N/A; The objective is to target a publication in *Science*. Dr. Epstein is familiar with an editor there and there is a good chance that it will get published. The projected timeline is late fall to mid next year and is dependent on the results of ongoing simulations.

External Conferences:

N/A; We are not currently targeting any external conferences.

Presentations at UTC:

K. Sreenivas, Research Dialogues 2019

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

The PI has ongoing collaborations with Drs. Mina Sartipi (Computer Science & Engineering, UTC) and Chandra Ward (Social Science, UTC) related to urban issues. This collaboration has resulted in two proposals, one each of NSF and the Lyndhurst Foundation. Additionally, new collaborations have been initiated with Drs. Yu Liang and Dalei Wu (Computer Science & Engineering) and that has resulted in a proposal to TDOT. Furthermore, the PI is already collaborating with Dr. Craig Tanis in an unrelated area; however, during discussions, the possibility of using Dr. Tanis's software for agent-based modeling was explored. This could lead to an in-house capability to have software agents react to various evacuation scenarios with further applications to spread of communicable diseases, urban transportation etc. An ongoing collaboration with Dr. Bathi (Civil & Chemical Engineering) has resulted in a pre-proposal to USGS.

EXTERNAL FUNDING

Proposal Submissions

1. Discovering Potential Reasons for Pedestrian Accidents, $205,152, TDOT, 02/06/2019
2. Preliminary Proposal: Smart Real-Time Control (SmaRT Control) for Accurate Monitoring and Management of Urban Stormwater Runoff, USGS, 02/15/2019
3. Exploring Transit Innovation in Chattanooga, $70,000, Lyndhurst Foundation, 07/12/2019
4. Data in GigCity: A Unified and Comprehensive Platform for Education and Research on Data Science and Engineering to Improve Accessibility in an Urban Environment, $2,912,891, NSF, 02/06/2019
5. Preliminary Proposal: NSF Engineering Research Center for Intelligent Connected Infrastructures in Sustainable Urban Environments (CONNECT), NSF, 01/16/2019

Contracts/Awards Received

1. CC* Compute: A Cost-Effective, 2,048 Core InfiniBand Cluster at UTC for Campus Research and Education, $392,235, NSF, 10/01/2019 – 09/30/2021
2. Heterogeneous HPC for High-Order Stabilized Finite-elements on Moving and Deforming Domains, SAIC Inc., $400,000, 09/01/2017 – 08/31/2019
3. Mesh curving for higher order applications, Pointwise Inc., $100,000, 06/01/2018 – 05/31/2020

Sponsored Program Capacity Building Activities

1. Ongoing monthly calls with Dr. Mike List, Air Force Research Laboratory, Wright Patterson Air Force Base, Ohio to discuss progress on research related to FUNSAFE.
2. Regular meetings with Dr. Steve Karman, Pointwise Inc., at the SimCenter to apprise him of the status on current funded research.
3. Met with NSF-Ignite program officers (on campus) to apprise them of current research areas related to urban issues.
4. Attended UTC's 1st Research Summit as the Department of Mechanical Engineering representative

WHAT'S NEXT FOR THIS RESEARCH?

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

Given the rapid urbanization of countries in both the developed and developing world, there are plenty of issues that need to be addressed. This will be carried out by collaborations with various faculty at UTC who have complementary skills. These collaborations have already resulted in multiple proposals and this will be pursued further.

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

The Energy and the Environment swimlane dovetails nicely with the work being carried out under the auspices of CUIP. As such, significant collaboration with Dr. Sartipi is already underway and is expected to continue. Additionally, collaboration with Dr. Bathi (Civil Engineering) will be pursued within the context of storm water management. Collaborations with

social scientists are also essential to address issues specific to urban areas and that will be pursued with Dr. Chandra Ward. Also of importance are the factors influencing transmission of diseases in a clinical setting. A collaboration with Dr. Henry Spratt (Biology) aimed at modeling the neo-natal ICU at Erlanger is being considered. This will result in a better understanding of the airflow patterns in the ICU and whether the location of the vents can be modified to minimize the spread of bacteria.

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?

The biggest barrier is time. Between the various responsibilities that a faculty member has, finding time during the semester to carry out significant research is limited. This could be alleviated through the use of graduate students, but finding good ones takes time.

FINANCIAL ACCOUNTING

The majority of the unspent funds came from the undergraduate student budget. While there were three undergraduate students working on this project at various times, they were unable to put in a lot of hours because of their schedules. Two of them were seniors and they were taking a considerable course load so that they could graduate in 4 years. Similarly, the junior who was working on the project also had a heavy course load which limited the time he could put into the project. Additionally, no publications have been produced directly from this research, so that part of the budget was also unspent.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Lead PI: Jin Wang

Co-PI(s): David Giles and Bradley Harris
Other Personnel: N/A

Project Title: Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation

Date Submitted: 07/31/2019

Award Start – End Date: July 1, 2018 – June 30, 2019

Non-Technical Summary:

The main objective of this project is to establish a new, experimentally guided, computational framework to investigate the fundamental pathogen dynamics associated with waterborne diseases. The project represents a pilot effort in the quantitative and systematic study of the pathogen dynamics associated with waterborne infections, integrating mathematical, computational and biological approaches. In particular, the computational framework bridges the pathogen dynamics at vastly different time scales in order to improve our current understanding of the exact roles played by the pathogens in shaping the complex epidemics and endemics of waterborne infections.

The project not only builds a solid knowledge base for understanding waterborne infection dynamics, but also provides useful public health guidelines for disease management and policy development. Meanwhile, the project enhances interdisciplinary curriculum development concerning the quantitative study of epidemiology and microbiology. Mentoring and training activities are centered on the graduate students involved in this project. Particularly, the project enhances the newly established Ph.D. concentration in Computational and Applied Mathematics at UTC. The project results in a number of journal publications, conference presentations, and external grant applications. Overall, the project contributes to the Capacity Building and Strategic Excellence in computational science at UTC and supports the mission of the SimCenter.

PROJECT TITLE: Waterborne Infections and Pathogen Dynamics: Modeling, Experimentation and Large-Scale Computation

Technology Area of Interest: Health/Biomedical Science

PROPOSED TECHNICAL APPROACH	OUTCOMES
The project integrates mathematical, computational and experimental methods to investigate waterborne pathogen dynamics. *List of tasks:* 1. Develop mathematical models for the environmental pathogen dynamics 2. Develop mathematical models for the within-host pathogen dynamics 3. Link and compute the between-host/within-host pathogen dynamics 4. Conduct laboratory experiments to guide, inform and validate models	An innovative mathematical and computational framework has been developed for the waterborne pathogen evolution in the environment and within the human body, and for the coupled between-host/within-host disease dynamics at different time scales. Project findings have been disseminated through journal publications and conference presentations. Results from this project have also contributed to several external grant applications. Two graduate students have been supported by this project.
RESULTS	**OTHER INFO**
(1) We have experimentally investigated and mathematically analyzed the Allee effects of the pathogenic bacteria. (2) We have measured, modeled and analyzed the bacterial growth dynamics under varied environmental conditions. (3) We have studied the bacterial-viral-immune interaction within the human body. (4) We have constructed new, multi-scale mathematical models that couple the within-host and between-host dynamics at different time scales. (5) We have conducted extensive numerical simulation to investigate the complex, nonlinear dynamics of waterborne infections.	**Budget and Schedule** Total Budget: $99,992.00 Actual Used: $83,865.21 Balance: $16,126.79 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-9 Task 3: Months 6-12 Task 4: Months 1-12 **Deliverables** • Final report detailing results, financials, and future work • Journal publications • External and internal conference presentations • External grant applications **Organization Information** *UTC Department of Mathematics* *425-4545*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Despite tremendous efforts on prevention and intervention programs and a large body of theoretical and clinical studies, waterborne infections remain a significant public health burden. Outbreaks related to waterborne diseases, such as cholera, have increased in severity, frequency and duration in recent years, indicating that our current knowledge and control strategies are inadequate. In particular, the dynamics of the waterborne pathogens, a critical factor in the epidemiologic triad of agent, host, and environment, are not well understood at present. For waterborne infections, the pathogen evolution often involves complicated ecological, biological, and physiological processes across a wide range of time scales, with multiple interactions taking place in the aquatic environment, among human hosts, and within the human body. This project conducts a pilot investigation into the complex, multi-scale pathogen dynamics, important for the control and management of waterborne diseases, through innovative modeling, careful experimentation, and advanced computation. The project integrates mathematical, computational, biological, and epidemiological methods, with biological experiments providing essential guidance, mathematical models laying the foundation of the study, scientific computation comprising the core of the investigation, and epidemiological data enabling important validation. This one-year project has generated some important findings, including the Allee effects of the pathogenic bacteria, the bacterial growth dynamics under varied environmental and physiological conditions, the bacterial-viral-immune interaction within the human body, and the mathematical and computational framework for modeling and connecting the between-host and within-host disease dynamics. These results contribute to the knowledge base of waterborne infections and their pathogen dynamics and could provide useful guidelines to public health administrations for effective disease prevention and intervention.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
1. Develop mathematical models for the environmental pathogen dynamics	Models are developed, analyzed and simulated, and are currently being refined.
2. Develop mathematical models for the within-host pathogen dynamics	Models are developed, analyzed and simulated, and are currently being refined.
3. Link and compute the between-host/within-host pathogen dynamics	Coupled between-host/within-host modeling framework has been developed and some computational results have been generated.
4. Conduct laboratory experiments to guide, inform and validate models	Experiments have been conducted and some important results have been produced.

Challenges & Strategies Used to Address / Overcome:

We have encountered a few challenges in the course of this research effort. These include: (1) We find that the between-host disease transmission could be impacted by a large number of factors, especially the distinctions of human hosts in different locations, the spatial movement of hosts and pathogens, the age structure of human hosts, and the environmental, geographical and socioeconomic conditions. We are currently extending our modeling framework to incorporate these factors. (2) The modeling of within-host disease dynamics is complicated by

the different types of host immune mechanisms. We are currently improving our models by distinguishing the innate immune response (which provides instantaneous, but short, protection of the body) and adaptive immune response (which provides delayed, but long-lasting, protection of the body). (3) In the experimental studies, the dose-dependent responses of the bacteria *V. cholerae* are difficult to observe under normal settings. To overcome this challenge, we have examined a wide variety of temperatures, salinity levels and pH values, and have reached extremely low levels of bacterial densities to reveal some important properties such as the Allee effects.

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

This project is centered on modeling and computation and is different from a typical hypothesis-driven biomedical project. Instead of proving/disproving a hypothesis, we combine mathematical modeling, experiments and scientific computation to investigate the complex dynamics of waterborne infections.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The project represents an interdisciplinary collaboration among Dr. Wang (an applied and computational mathematician), Dr. Giles (a microbiologist), and Dr. Harris (a bioengineer). Dr. Wang is a full professor and this project provides new avenues for his research endeavor, particularly to apply his mathematical models and computational methods to a realistic problem with high importance in public health. Drs. Giles and Harris are younger faculty members and this project provides a valuable opportunity to advance their research careers. Overall, each of the PI and Co-PIs has benefited from the research experience and the interdisciplinary collaboration through this project.

Students Impacted

Conrad Ratchford is a PhD student in the Department of Mathematics. With the support from this project, he has generated solid results in mathematical and computational modeling of waterborne infectious diseases and is making good progress toward his PhD.

Erick Rojas is a graduate student in the Department of Chemical Engineering. With the support from this project, he has performed important experimental studies and successfully completed his M.S. degree in June 2019.

In addition, the project has impacted several other students who conducted related research; these include PhD student Chayu Yang in the Department of Mathematics, and undergraduate student Eric Siv in the Department of Biology and Environmental Science.

Community and Broader Impacts

Waterborne infections represent a serious public health threat, with several millions of cases reported each year. Results from this project improve our understanding on the persistence of waterborne infections, quantification of individual disease risk, and relationship between individual pathogen burden and population-level disease transmission. As such, the project

findings can provide useful guidelines to public health administrations for disease management and policy development.

Scholarly Products

Publications*:*

C. Ratchford and **J. Wang,** "Multi-scale modeling of cholera dynamics in a spatially heterogeneous environment." Under review (for journal publication), 2019.
K. Yamazaki, C. Yang and **J. Wang,** "A partially diffusive cholera model based on a general second-order differential operator." Under review (for journal publication), 2019.
J. Yang, C. Modnak and **J. Wang,** "Dynamical analysis and optimal control simulation for an age-structured cholera model." Under review (for journal publication), 2019.
J. Bai, C. Yang, X. Wang and **J. Wang**, "Modeling the within-host dynamics of cholera: Bacterial-viral-immune interaction." Under review (for journal publication), 2019.

External Conferences*:*

Jin Wang, "Modeling and simulating cholera dynamics, Computational and Applied Mathematics Colloquium," Pennsylvania State University, October 2018.
Jin Wang, "Analyzing the within-host dynamics of cholera, Special Session on Differential Equations in Mathematical Biology," AMS Spring Southeastern Sectional Meeting, Auburn, AL, March 2019.
Eric Siv, Erick Rojas, **David Giles**, **Bradley Harris**, and **Jin Wang**, "An Examination of Allee effects in Vibrio cholera," The 80th Annual Meeting of ASB, Memphis, TN, April 2019.

Chayu Yang and **Jin Wang**, "Modeling the within-host dynamics of cholera, UTC Research Dialogues," April 2019.
Jin Wang, "Mathematical modeling of infectious diseases, Biology Seminar," University of Tennessee at Chattanooga, April 2019.
Erick Rojas, "Determination of Allee Effects and Virulence in Vibrio Cholerae," M.S. (in Engineering) thesis defense, June 2019.
Jin Wang, "Infectious disease models and differential equations," Department of Mathematics, University of Tennessee at Chattanooga, June 2019.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

This project stimulates and enables new collaborations with researchers at several other universities, including Dr. K. Yamazaki at Texas Tech, Dr. L. Mu at University of Georgia, and Dr. J. Chen at University of Virginia. Some of these research collaborations have already generated meaningful results and produced preprints.

EXTERNAL FUNDING

Proposal Submissions

1. NSF REU program: proposal submitted in August 2018 (PI: A. Ledoan; co-PI: J. Wang)
2. NSF Math Biology program: proposal submitted in September 2018 (PI: J. Wang)
3. NIH R15 program: proposal submitted in October 2018 (PI: J. Wang; co-Is: Giles & Harris)
4. NSF Computational Math program: submitted in December 2018 (PI: E. Panagiotou; co-PI: J. Wang)

Contracts/Awards Received

1. REU Site: Research Training for Undergraduates in Mathematical Analysis with Applications in Allied Fields. PI: Andrew Ledoan; Co-PI: Jin Wang. National Science Foundation (REU program), 2019–2022, $282,659.
2. Computational Methods for Measuring Topological Entanglement in Polymers. PI: Eleni Panagiotou; Co-PI: Jin Wang. National Science Foundation (Computational Math program), 2019–2022, $125,000.
3. Experimentally Guided Modeling and Simulation for Cholera Dynamics. PI: Jin Wang; Co-Is: David Giles and Brad Harris. National Institute of Health (R15 program), 2019–2022, $340,000.

Sponsored Program Capacity Building Activities

1. Communicated (through emails, phone calls and face-to-face meetings) with NIH program officers Dr. David Filpula and Dr. Ravi Veerasamy.
2. Attended the MIDAS (Models of Infectious Disease Agents Study) network meeting and workshop sponsored by NIH in May 2019.

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 the research efforts in modeling and computing waterborne infections. We plan to expand the modeling techniques to include stochastic approaches which would involve stochastic differential equations and Monte Carlo simulation, and which would better catch the random effects in disease epidemics. We also plan to combine our current mathematical and computational methods with machine learning techniques in order to design next-generation, data-driven modeling framework for waterborne infectious diseases.

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

With the support from CEACSE, this pilot project has opened up opportunities for several related research efforts. For example, the modeling and computational framework developed in this project can be extended to the study of other types of infectious diseases. Meanwhile, the holistic modeling approach employed in this project, which integrates mathematical, computational and experimental methods, can be applied to the investigation of many other

problems in biological and medical sciences. We plan to expand our collaboration to people in statistics, computer science, and public health in pursuing these future research efforts.

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

Some funds (about $16,126.79) remain at the end of the project, mainly because the PI budgeted 0.75 months additional pay (and related fringe benefits) for the month of June 2019 but that payment did not go through. The PI communicated this issue with Dr. Tony Skjellum, Anna Lane and Virginia Moore.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

NAME, Lead PI: Weidong Wu

Co-PI(s): Jejal Reddy Bathi

Project Title: Modeling Fate and Transport of Engineered Nanomaterial in Surface Water Systems

Date Submitted: 8/26/2019

Award Start – End Date: July 1, 2018 – June 30, 2019

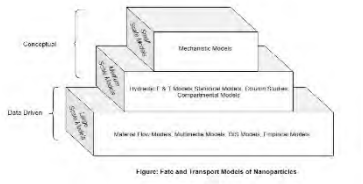
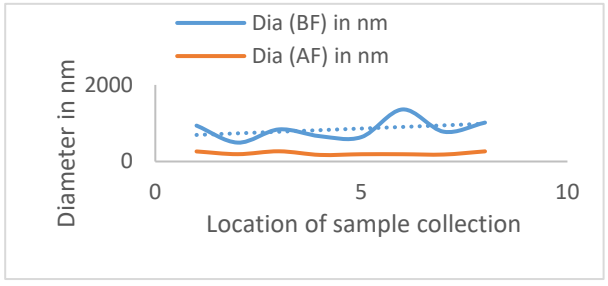
Non-Technical Summary:

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 using fate simulation models. There are no reliable fate models that currently available have proven the ability to simulate ENM behavior in the environment. As part of our research, we reviewed generally used water quality simulation models and their applicability to model ENMs in surface waters. Since the literature pertaining to type and quantity of ENM in the surface water environment is limited, as the first phase of the proposed research, a systematic evaluation of available literature to identify prominent ENMs and their physical, chemical, and biological properties that are important in pollutants fate assessment was conducted. Second and third phases of the proposed research were to develop a calibrated EFDC model for river hydraulics and ENM fate simulation.

The research findings provided a demonstrated case study to present at the local national conference. The research findings were published as conference proceedings and as a book chapter in addition to several student posters and podium presentations at the technical conferences. The research findings were are also aided in the development of external funding proposal.

PROJECT TITLE

Technology Area of Interest: Energy and the Environment

PROPOSED TECHNICAL APPROACH	OUTCOMES
• Compilation of physiochemical properties of ENMs that can be used to model fate and transport of the ENMs in surface waters. • Set-up and calibrate a hydrodynamic model for water quality simulation	• Identified and compiled primary properties of interest for determining the fate and transport of ENMs • Developed preliminary field data of nanomaterials • Findings are published as posters, podium presentations, and conference proceedings
RESULTS	**OTHER INFO**
A detailed review of available/potential models for fate modeling is conducted. The models are primarily categorized into Conceptual and Data-Driven. Also a preliminary numerical model is being set up.  In coordinated efforts of our work on United States Geological Survey (USGS) 104(b) research project, our CEACSE research efforts have led to the development of A MATLAB based structured grid generator for EFDC model and compatibility test of our new grid generator tool is found satisfactory. Figure 2. Illustration of our field measure nanomaterial (NM) distribution in the Tennessee River of our proposed model domain.  Figure 2. NM distribution in TN River	**Total Project Budget: $96,217.00** **Balance Budget: $5,287.12** **Organization Information** Civil and Chemical Engineering

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The overall objective of the proposed research was to build upon on-going research to develop a 3-dimensional hydrodynamic model to simulate fate and transport of emerging contaminants of Engineered Nanomaterials (ENMs). The proposed research project was a demonstration study to showcase the use of 3D modeling to assist regulators, watershed management agencies, municipalities and utilities in life cycle analysis of ENM and help sustain urban waterways. Most importantly, the proposed research was able to provide research opportunities for both undergraduate and graduate students and help develop concept demonstration data for seeking external funds for future research in computational applications in the water resources and environmental engineering arenas.

The approach of the research was to start with identifying and developing parameters of interest of ENMs to determine their fate and transport in surface water systems. A parallel task of the research was to evaluate the potential use of existing simulation programs for simulating the ENMs fate and transport. An independent task, in coordinated efforts with ongoing USGS 104(b) funded research, was to develop a calibrated EFDC hydrodynamic model that then can be tested for simulating the fate and transport of the ENMs.

The project has conducted an extensive, detailed review of the literature and identified the most prominent ENMs and their parameters and properties of water media that are key in determining fate and transport of the ENMs in surface waters. In addition, the project team has developed EMMs key parameters data by collecting and analyzing field samples and also using synthetic samples. While the EFDC model is being tested for simulating fate and transport of ENMs in surface waters, a new grind generator tool has been developed and tested.

Findings of the research were presented both at local and national level conferences. In addition, research findings provided seeding data to seek external funding. Both grad and undergrad students were trained on the research aspect of water quality simulation, environmental field sampling, and laboratory chemical analysis.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Gather ENM fate model set-up data	Significant data to test fate and transport of ENMs is compiled
Review and evaluate (test) applicability of simulation models for ENMs fate modeling	An extensive review of simulations models for the ENMs fate modeling was completed. A manuscript draft of review findings is being developed.
With the coordinated research efforts with USGS 104(g) research project, build and test EFDC model for ENMs fate simulation	EFDC model is being developed that is suitable to test its applicability for ENMs fate and transport.

Student development	There were two graduate students (MS Civil Engineering), two undergrad students (BS in Civil Engineering) and one undergrad student (BS in Chemical Engineering) trained on the research in ENMs fate and transport.
Development of scholarly products	There are several poster and conference presentations and book chapter publications were developed. Additional journal manuscripts are being developed.
External Funding	Outcomes of the research have partially helped submitting a research proposal to USGS 104(g). The seeding data developed from this project is expected to yield additional future proposals.

Challenges & Strategies Used to Address / Overcome:

The primary challenge of the project was establishing a three-dimensional grid to use with the EFDC model. The grid generated program available with EFDC is no longer available and we explored the use of other similar programs. However, those programs were either proprietary or found not capable of generating a compatible grid to use with the EFDC model. To deal with the issue, an in-house grid generator program was developed and tested. This provided additional tools and a new outcome from the research.

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

The project was set to work in coordination with research efforts of another funded project (USGS 104(b)), where one of the tasks of the project is to test calibrated EFDC hydrodynamic model for ENMs fate and transport simulation. However, the delayed start date of USGS 104(b) project has limited the opportunity to fully develop a calibrated hydrodynamic model. Hence the testing of applicability of EFDC for ENMs fate simulation was not successfully demonstrated. Meanwhile, the project team has reviewed several other models and their approaches for potential use and limitations for modeling fate and transport of the ENMs in surface waters.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The research funding has provided early-career faculty with the ability to build their capacities to support tenure opportunity (Dr. Wu) and prepare for a future tenure-track faculty position in engineering (Dr. Bathi).

Students Impacted

Shuvashis Roy, MS in Civil Engineering, expected graduation December 2019

Syed Tareq, MS in Civil Engineering, expected graduation December 2019

Patrick Craig, BS in Civil Engineering, expected graduation December 2020

Jenk Parker, BS in Civil Engineering, expected graduation May 2020

Haiven Camenisch, BS in Chemical Engineering, Junior.

All these students were exposed and trained in the area of ENM pollution, analysis, and data analysis. Graduate students working on the project also developed part of their graduate thesis report.

Community and Broader Impacts

The research has potential multiple impacts. Most notably, a calibrated hydrodynamic and water quality model is a good demonstration to help local stakeholders such as water utilities, public work agencies, and regulatory make an informed decision about how to manage the water resources. Proposed models provide tools for integrated management of urban water resources. For example, with the application of this model, water utilities can understand the receiving water quality, both spatially and temporally, and make decisions accordingly for drawing water such that they can optimize the water treatment processes and provide clean water to customers in a more cost-effective manner.

The research findings were presented both at local and national level events that are focused on water management. For example, research work presented at the 2019 Chattanooga Development Symposium has well demonstrated our river modeling and its potential use for the municipal and other regulatory stakeholders.

Scholarly Products

Book Chapter:

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

External Conferences:

Bathi., **J**.**R**., Clark., S., Gadhamshetty., V., Tareq., S., Roy., S. “Characterization of Polycyclic Aromatic Hydrocarbons and Engineered Nanomaterial in Surface Water Environment” ASCE Environmental and Water Resource Institute (EWRI) Conference, Pittsburgh May 2019. (Conference proceedings)

Bathi., **J**.**R**., Geza., S., Gadhamshetty., V. “Emerging Water Infrastructure: Occurrence and Treatability aspects of Engineered Nanomaterial” ASCE Environmental and Water Resource Institute (EWRI) Conference, Pittsburgh May 2019. (Podium presentation)

Roy., S., **Bathi**., **J**. **R**. “Decision Supporting Hydrodynamic Modeling of TN River,” 28th Tennessee Water Resources Symposium, Montgomery Bell State Park, Burns, TN, August 06, 2019 (Poster)

Bathi., **J.R**., Clark., S., Tareq., S., Roy., S., Gadhamshetty., V. “Characterization of Polycyclic Aromatic Hydrocarbons and Engineered Nanomaterial in Surface Water Environment” ASCE Environmental and Water Resource Institute (EWRI) Conference, Pittsburgh May 2019. (Podium presentation)

Roy., S., **Bathi**., **J**. **R**. “Decision Supporting Hydrodynamic Modeling of TN River,” 28th Tennessee Water Resources Symposium, Montgomery Bell State Park, Burns, TN, April 10-12, 2019 (Poster).

Tareq., S., **Bathi., J. R.** “Characterization of Nano Contamination: Challenges and Findings” University of Tennessee Research Dialogues, April 10, 2019 (Poster)

Bathi, J.R., Tareq., S., Palchoudary., S. “Detection and Treatability of Nanomaterial in Surface Waters,” 28th Tennessee Water Resources Symposium, Montgomery Bell State Park, Burns, TN, April 10-12, 2019 (Podium Presentation)

Presentations at UTC:

Roy., S., Bathi., J. R. “Decision Supporting Hydrodynamic Modeling of TN River,” University of Tennessee Research Dialogues, April 10, 2019 (Presentation)

Tareq., S., **Bathi., J. R**. “Characterization of Nano Contamination: Challenges and Findings” University of Tennessee Research Dialogues, April 10, 2019 (Poster)

Craig., P., Sawyer., S., **Bathi., J.R**. “Nanomaterial: Characterization and Treatment in Urban Stormwater Runoff” University of Tennessee Research Dialogues, April 10, 2019 (Poster)

Proposed Journal Articles:

It is intended that this work will be submitted for publication to Journal of Contaminant Hydrology and journal of Environmental Science & Technology. Expectations are initial submission should take place in later part Fall 2019 and Spring 2020.

Tentative Article Name:

1. Modeling Fate and Transport of Engineered Nanoparticles in surface water
2. Understanding fate and transport of engineered nanoparticles in surface water using a 3D hydrodynamic procedure

Inventions or Other Intellectual Property

None

Research Outreach & Collaboration

Collaborated with faculty at South Dakota School of Mines and Technology on the analysis and treatment of ENMs

EXTERNAL FUNDING

Proposal Submissions

Fate and Transport of Engineered Nanomaterial in a River System, Funding Agency: U.S. Geological Survey, through Tennessee Water Resources Center, Total Budget: $25,000 external (USGS) + $50,000 (internal, UTC match) (Un-funded)

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?

Plans are set in place to continue to explore the research in the topic area. More specifically, in two major sections:

1. Development of standard methods for environmental sample collection analysis for ENMs evaluation in surface waters
2. Analysis and development of bioretention based treatment techniques for ENMs treatment.

Currently, the seeding data developed as part of the CEACSE fund is being used to put together a proposal to be submitted to NSF.

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

We are currently seeking research funding from USGS and NSF. We have plans in place to request funding from the United States Department of Agriculture in the area of simulating nano pollution control in agricultural farms.

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

None

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

Continue to support grad students through their degree completion which is essential for developing research proposals based on seeding data that has been developed.

FINANCIAL ACCOUNTING

Since the project is not confirmed and started late in Spring/Summer, it became challenging to recruit graduate students, plan research activities, and acquire research resources, including equipment, in time.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Michael Danquah, Lead PI

Other Personnel: None

Project Title: Kinetic and computational elucidation of nucleic acid aptameric binding mechanism for enhanced molecular targeting

Date Report Submitted: August 15, 2019

Award Start – End Date: August 15, 2018 – June 14, 2019

Non-Technical Summary:

This project studied the fundamental molecular mechanisms responsible for the functionality of DNA aptamers as biomolecular probes for diagnostics and targeted delivery applications. Specifically, the project investigated the biophysical binding process and structural transformations of DNA aptamers via molecular dynamics modeling and simulation using a thrombin-binding aptamer (TBA) as a model. This molecular-level modeling and simulation offered real-time analysis and visualization of TBA-thrombin binding process and was significant in determining relevant TBA conformations and conditions for enhanced thrombin binding. We successfully modeled the TBA-thrombin structures for molecular dynamics (MD) simulations to determine the molecular features of the binding process and stability.

The mini-CEACSE FY19 funding served as important seed funding to build research capacity in the area of aptamer-target binding for theranostic applications. Specifically, it has contributed in developing the initial research work that will form the foundation of building a stronger research program through the pursuance of external research funding, expanding research facilities, recruiting graduate and undergraduate research students, increasing research publications and developing intellectual properties, engaging with the community and expanding collaborative supports. The mini-CEACSE FY19 funding resulted in the following achievements (i) 3 external research proposals submitted to National Science Foundation, St. Baldrick Foundation, and Prevent Cancer Foundation; (ii) recruitment of 2 undergraduate students to work on the project – promoting experiential learning via research training, (iii) participation in 2019 UTC research dialogue and CECS Tech Symposium, (iv) 3 research manuscripts; all under review with Chemical Engineering Journal, Scientific Reports and Biotechnology Advances, and (v) strengthening collaborations with internal and external partners. These outcomes directly advance the mission of SimCenter particularly in the area of using computational engineering tools for biomedical applications in disease diagnosis, pathogen detection, and targeted delivery of cancer.

PROJECT TITLE

Technology Area of Interest: Health and Biosystems

PROPOSED TECHNICAL APPROACH

The project investigated the biophysical binding process and structural transformation mechanisms of DNA aptamers via molecular dynamics modeling and simulation using a thrombin-binding aptamer (TBA) as a model.
Task 1 – Structural modeling of TBA and thrombin protein
Task 2 – MD simulation of TBA-thrombin binding to investigate changes in TBA structural conformation and binding stability.

OUTCOMES

We successfully modeled the TBA-thrombin structures for molecular dynamics (MD) simulations to determine the molecular features of the binding process and stability.
Task 1 – The configuration of the aptamer was modeled from the X-ray crystallography structure in the presence of K^+ with PDB entry 5CMX.
Task 2 – MD simulation and free-energy profiling of thrombin binding by 31-mer TBA aptamer in a water box was achieved.

RESULTS

Fig 1 shows the MD simulation and free-energy profile of thrombin binding by a thrombin-binding 31-mer aptamer in a water box. The configuration of the aptamer was taken from the X-ray crystallography structure in the presence of K^+ with PDB entry 5CMX. Na^+ and Cl^- were added to balance the net charge at 0.1 M concentration. MD simulation was performed under an NPT ensemble (1 atm and 300K) and periodic boundary conditions. To bind to thrombin, the aptamer folded into two G-quadruplex (G4) motifs and stabilized by the metal cation K^+ (or Na^+) (Fig. 1A). Free energy (potential of mean force, PMF) simulation was performed (Fig. 1B) using the distance between the center of mass of a flexible loop and that of the aptamer (Fig. 1C) as the reaction coordinate (RC), and the configuration with the minimal free energy was located at RC = 10.7 Å. The free energy simulations provided insights into the stability

OTHER INFO

Budget and Schedule

Total Budget:	$14,976.00
Actual Used:	$11,925.45
Balance:	$ 3,050.55

Total period of performance is 9 months.
Task 1: Months 1-4
Task 2: Months 5-9

Deliverables

- Final report detailing results, financials, and future work
- External research funding applications
- Publications
- Internal conference presentation

Organization Information

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Department of Civil & Chemical Engineering
615 McCallie Ave, Chattanooga,
TN 37403, United States
Phone: 423-425-4096
Email: michael-danquah@utc.edu

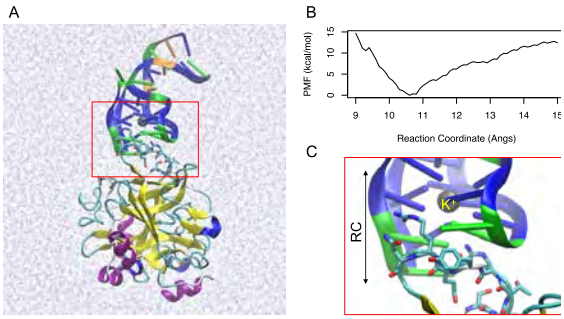


Fig 1. (A) Aptamer-thrombin complex in a water box for MD simulations. The system contains 113,967 atoms, including 36,126 H_2O (blue sticks), 94 Na^+, 68 Cl and an 31-mer aptamer 5'-GTGACGTAGGT TGGTGTGGTTGGGGCGTCAC-3'.(B) Free energy (potential of mean force) profile of the aptamer-thrombin binding process using the distance between center of mass of a flexible loop with that of the aptamer as the reaction coordinate (RC). (C) The loop region inserts (zoomed from A) into the thrombin under the two guanine (blue) quadruplexes that were stabilized by a potassium ion (black spheres).

ACCOMPLISHMENTS & OUTCOMES

Project Overview

An efficient real-time biomolecular binding mechanism is urgently needed to rapidly detect and isolate disease pathogens and biotoxins from water bodies, soil, food samples, and body fluids. Aptameric binding is a unique biological phenomenon for probing a wide range of cellular and (bio)molecular targets. Aptamers are single-stranded oligonucleotides with affinity binding mechanisms effective for selective and specific identification of cellular and non-cellular targets. The degree of binding specificity is driven by unique transformations in their structural and hydrodynamic conformations resulting from ionic charge distribution of the target molecule. However, the theoretical underpinnings of aptameric binding behavior and molecular mechanisms governing the structural folding for target binding specificity is limited. This has obstructed advancements in the utilization of this phenomenon for innovative biosensing applications. This project will study the biophysical binding mechanism of nucleic acid aptamers and investigate structural transformation mechanisms and binding motifs via molecular dynamic modeling in order to build the theoretical framework important to optimize binding performance for tailored applications. Such a molecular-level modeling, offering real-time analysis and visualization of the binding process, would be significant in molecularly engineering the binding characteristics of aptamers towards specific targets.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Structural modeling of TBA and thrombin protein	40%: The configuration of the aptamer was modeled from the X-ray crystallography structure in the presence of K^+ with PDB entry 5CMX.
MD simulation of TBA-thrombin binding to investigate changes in TBA structural conformation and binding stability	100%: MD simulation and free-energy profiling of thrombin binding by 31-mer TBA aptamer in a water box was achieved.

Challenges & Strategies Used to Address / Overcome:

An obstacle encountered in the beginning of the project relates to delays in the recruitment of suitable students to work on project. This however, did not affect the achievement of project objectives.

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

None

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The mini-CEACSE FY19 funding served as an important seed funding for the PI to rapid progressions in building his research in the area of aptamer-target binding for theranostic applications at UTC. Specifically, it has contributed in developing the initial research work that will form the foundation of building a stronger research effort in this area through the pursuance of external research funding, expanding research facilities, recruiting graduate and undergraduate research students, increasing research publications and developing intellectual properties, engaging with the community and expanding collaborative support.
The mini-CEACSE FY19 funding resulted in the following achievements (i) 3 external research proposals submitted to National Science Foundation, St. Baldrick Foundation, and Prevent Cancer Foundation based on findings from this work; (ii) recruitment of 2 undergraduate students to work on the project in order to promote research training, (iii) participation in 2019 UTC research dialogue and CECS Tech Symposium, (iv) 3 research manuscripts; all under review with Chemical Engineering Journal, Biotechnology Advances and Scientific Reports, and (v) strengthening collaborations with internal and external partners. These outcomes directly advance the mission of SimCenter particularly in the area of using computational engineering tools for biomedical applications such as disease diagnosis, pathogen detection, and targeted delivery of cancer.

Students Impacted

Mikayla Hawkins, undergraduate student Chemical Engineering. The mini-CEACSE funding and supported the student and promoted research training and experiential learning. The student gained hands-on research experience in structural modeling and molecular dynamics simulation

with applications in apta-targeting of cancer receptors. The student presented a poster at 2019 Research Dialogue and CECS Tech Symposium.

Alexis Hartwig, undergraduate student, Chemical Engineering. The mini-CEACSE funding and supported the student and promoted research training and experiential learning. The student gained hands-on research experience in structural modeling and molecular dynamics simulation with applications in apta-targeting of cancer receptors. The student presented a poster at 2019 Research Dialogue and CECS Tech Symposium.

Community and Broader Impacts

The mini-CEACSE funding laid the foundation for the PI's collaboration with Erlanger hospital. The PI is currently working with Dr. Manoo Bhakta (Erlanger hospital, Chattanooga) to develop an enhanced aptamer-based CD19 receptor binding mechanism for acute lymphoblastic leukemia treatment.

Scholarly Products

Publications:

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

1. Caleb Acquah, Yi Wei Chan, Sharadwata Pan, Lau Sie Yon, Clarence M. Ongkudon, Haobo Guo, **Michael K**. **Danquah**." Aptamer-anchored poly(EDMA-co-GMA) monolith for high throughput affinity binding." Scientific Report (under review)
2. Jaison Jeevanandam, Kei X. Tan, **Michael**. **K**. **Danquah**, Haobo Guo, Andrew Turgeson. "Advancing aptamers as molecular probes for cancer theranostic applications – the role of molecular dynamics simulation." Biotechnology Advances (under review)

Presentations at UTC:

1. **Michael K Danquah**, Haobo Guo, Mikayla Hawkins, Alexis Hartwig. "Engineering aptamer-mediated targeted cancer therapy." Poster presentations. 2019 UTC Research Dialogue and CECS Tech Symposium.

Inventions or Other Intellectual Property

None

Research Outreach & Collaboration

Through the mini-CEACSE funding, the PI has built collaborations with Dr. Manoo Bhakta (Erlanger hospital, Chattanooga), Dr. Guo Haobo (UTC SimCenter), Dr. Bradley Harris (UTC, Chemical Engineering), Dr. Soubantika Palchoudhury (UTC, Chemical Engineering) Dr. David Levine (UTC, Physical Therapy) and Dr. Henry Spratt (UTC, Biology).

EXTERNAL FUNDING

Proposal Submissions

1. Atomistic probing of CD79 apta-marking for enhanced pre-B-ALL diagnosis. Submitted to Prevent Cancer Foundation. $100,000.00. PI: Dr. Danquah & co-PI: Dr. Harris.
2. A portable paper-based aptasensor for rapid and simultaneous detection of multiple food and water-borne pathogens. National Science Foundation. $340,084. PI Dr. Danquah; co-PIs Drs Spratt, Levine and Giles
3. Aptameric targeting of CD19 transmembrane receptors for Acute Lymphoblastic Leukemia therapy. Submitted to St. Baldrick Foundation. $92,240.00. PI: Dr. Danquah & co-PI: Dr. Manoo Bhakta (Erlanger).

Contracts/Awards Received

Aptameric targeting of CD19 B-lymphocyte transmembrane receptor via molecular dynamics simulations for acute lymphoblastic leukemia therapy.

UTC-UTCOM-Erlanger Collaborative Grant: $25,000.00

Dr. Michael Danquah (UTC PI) and Dr. Manoo Bhakta (Erlanger PI)

Sponsored Program Capacity Building Activities

I have attended a number of on-campus funding and grantsmanship workshop organized by ORSP and SimCenter.

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 couple of years, I wish to focus on pursuing external and internal funding to support my research on bioaffinity targeting for theranostic applications. The findings from the mini-CEACSE project has already formed the basis of 3 external funding applications.

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?
Related research focus will be on environmental applications of bioaffinity systems for pathogen detection through collaborations with Dr. Henry Spratt (UTC, Biology) and Dr. David Levine (UTC, Physical therapy)

Tell us anything else we should know about this work not described above.
None

What barriers (if any) do you face to reach these next goals?
None

FINANCIAL ACCOUNTING

Funds were budgeted to cover publication cost but were not used since all our manuscripts are still under review. In addition, due to the delay in the recruitment of a student for the project, part of the funds budgeted for salary/fringe benefits were not used.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Francesca Leasi, Lead PI

Other Personnel: None

Project Title: “Development and application of bioinformatics pipelines and theoretical models to predict microbiome biodiversity in response to environmental stressors”

Date Report Submitted: August 15**,** 2019

Award Start – End Date: August 15, 2018 – June 14, 2019

Non-Technical Summary:

The main goal of the project was to build bioinformatics pipelines and environmental models to assess and predict biodiversity of microscopic organisms under environmental stressors. I am a junior faculty who started a tenure-track position in Fall 2018. In line with the main missions of the SimCenter, the mini-CEACSE grant allowed me to immediately establish collaborations with faculty at UTC. In this context, I have submitted an interdisciplinary grant proposal to the CEACSE program with other faculty at UTC from different departments. The proposal has been funded to promote outreach activities by organizing the First Southeastern Computational School. The workshop was very successful and attracted 25 among students and faculty from UTC and other 14 different institutions. I also used the grant to support one undergraduate and one graduate student in computer science. This grant allowed me to enhance knowledge in computational biology at UTC. Attending such a workshop allowed me to improve skills in computational biology and achieve familiarity with the main tools. In this context, I have computationally analyzed data and obtained results that were presented at an international conference. The grant also allowed me to get preliminary data that are being used to prepare an extra-mural fund grant proposal.

PROJECT TITLE: Development and application of bioinformatics pipelines and theoretical models to predict microbiome biodiversity in response to environmental stressors
Technology Area of Interest: Energy and the Environment & Health and Biosystems

PROPOSED TECHNICAL APPROACH	OUTCOMES
• Most of the project has been focused on organizing outreach in a form of a computational workshop. • The grant greatly helped to computationally analyze data.	The workshop has been filled with 25 attendees from 15 institutions The analyzed data were presented in form of oral communication at the international meiofauna conference, Evora (Portugal) July 7–12, 2019. Leasi et al. Integrating biodiversity surveys of meiofauna and microbiome for ecosystem biomonitoring
RESULTS	**OTHER INFO**
	Budget and Schedule Total Budget: $19.905 Actual Used: $19.905 Balance: $ 0 Total period of performance is 6 months. Task 1: Months 1-6. Workshop organization and data analyses. **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. *Results obtained from a previous research were analyzed.* • Final report detailing results, financials, and future work. *Results allowed me to obtain preliminary data to prepare an extra-mural grant proposal.* • External and internal conference presentation. *International meiofauna conference, Evora (Portugal) July 7–12, 2019. Leasi et al. Integrating biodiversity surveys of meiofauna and microbiome for ecosystem biomonitoring*

ACCOMPLISHMENTS & OUTCOMES

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Organize computation workshop	25 among students and faculty from UTC and other 14 different institutions attended the workshop.
Analyze data previously acquired computationally	Results have been presented in an international conference. A peer-reviewed publication based on such results is currently in preparation

Challenges & Strategies Used to Address / Overcome:

The original proposal included an articulated research project, which was not pursued due to the delay in my research lab construction. The lab was made available to me only in May 2019 instead of August 2018. However, I was fortunate to be allowed to make significant changes in the budget and use the grant proposal to organize the computational workshop.

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

Once I redirected the budget, things worked pretty smoothly and successfully.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

N/A

Students Impacted

N/A

Community and Broader Impacts

N/A

Scholarly Products

Publications:

N/A

External Conferences:

Leasi et al. Integrating biodiversity surveys of meiofauna and microbiome for ecosystem biomonitoring. International Meiofauna Conference. Evora (Portugal) July 7-12, 2019.

Presentations at UTC:

N/A

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

N/A

Contracts/Awards Received

N/A

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?

N/A

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

N/A

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

N/A

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Jared A. Pienkos, Lead PI

Other Personnel: N/A

Project Title: Exploiting Alkynyl Titanocenes for Carbon-Carbon Bond Formation

Date Report Submitted: 8/3/19

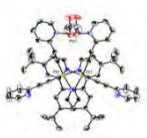
Award Start – End Date: August 15, 2018 – June 14, 2019

Non-Technical Summary:

Our project focused on the design of ligands, or compounds that bind to metals, which are typically utilized to modulate the reactivity of catalysts. We were able to successfully design, synthesize, and characterize one of these said ligands. During the course of this study, eight undergraduate students were trained in synthetic chemistry, and basic programs were utilized with computational chemistry. Five of these students will present work at SERMACS, a regional chemistry conference. Two of these students provided outreach activities to a group of home-schooled students and to a local private high school. We believe these activities are in line with the SimCenter's mission to integrate education and research, as multiple students and members of the community were impacted by this project.

PROJECT TITLE: Exploiting Alkynyl Titanocenes for Carbon-Carbon Bond Formation
Technology Area of Interest: N/A, Mini-CEACSE

PROPOSED TECHNICAL APPROACH	OUTCOMES
• Synthesize and characterize new trans-bidentate ligands, and computationally model these compounds. • Generate outreach programs based on computational modeling.	We synthesized and characterized the ligand tBpyPt(C22py)2 and characterized its interactions with Cu(I) and Pd(II) salts. We provided the community with two successful outreach activities.

RESULTS	OTHER INFO
An example of the tBpyPt(C22py)2 ligand's interaction with Pd(II). This is through a continued collaboration with Clemson University's crystallographer.  See supplemental letters 1 and 2 for proof of community impact.	**Budget and Schedule** Total Budget: $14,999 Actual Used: $14,641.92 Balance: $ 357.08 **Organization Information** Jared Pienkos 320 Grote Hall, Dept 2252, 615 McCallie Ave, Chattanooga, TN 37403. 732–513–2644, Jared-pienkos@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

We synthesized ^{t}bpyPt($C_2$2-py)$_2$ (Figure 1, Compound 1), and investigated its interactions with Pd(II) and Cu(I) salts. The metalloligand ^{t}bpyPt($C_2$2-py)$_2$ was synthesized in two steps (Figure 1). (1) Refluxing K_2PtCl_4 with ^{t}bpy in the presence of HCl produced ^{t}bpyPtCl_2.

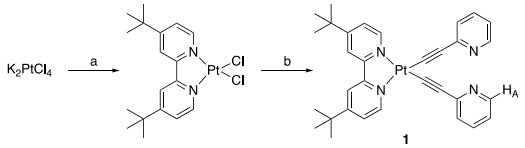


Figure 1: Synthesis of Metalloligand

(2). Using a modification of the procedure reported by Lu et al., ^{t}bpyPt($C_2$2-py)$_2$ (**1**) could be synthesized in a 91.1% yield. Pd(II) complexation with the ^{t}bpyPt($C_2$2-py)$_2$ metalloligand was obtained by treating an arene solution of ^{t}bpyPt($C_2$2-py)$_2$ with Pd(OAc)$_2$. For instance, treating a benzene-d_6 solution of ^{t}bpyPt($C_2$2-py)$_2$ with Pd(OAc)$_2$ showed an immediate change (^{1}H-NMR). The sole ^{t}bpy resonance (1.22 ppm) present in ^{t}bpyPt($C_2$2-py)$_2$ became two peaks (1.16 ppm and 1.15 ppm) upon Pd(II) coordination, which indicates a lesser degree of symmetry in the Pd(II) bound complex compared to ^{t}bpyPt($C_2$2-py)$_2$.

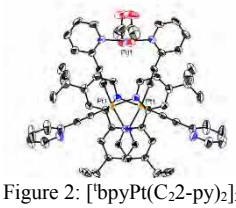


Figure 2: [^{t}bpyPt($C_2$2-py)$_2$]$_2$Pd(OAc)$_2$

This is also highlighted in the aromatic region of the Pd(II) complexed species where there are a total of fourteen inequivalent hydrogens.

X-ray analysis of the Pd(II) bound species indicated that one equivalent of $Pd(OAc)_2$ complexed with two equivalents of ^{t}bpyPt($C_2$2-py)$_2$, which formed [^{t}bpyPt($C_2$2-py)$_2$]$_2$Pd(OAc)$_2$ (Figure 2). The two Pt-pyridyl derivatives are bound *trans* to one another, likely due to a steric strain that would be caused if these ligands were in the *cis* confirmation.

To investigate the structural differences between **1** and previously reported ligands, DFT calculations were performed. For the Pt-metalloligand, a B3LYP basis set was utilized with cc-pVDZ basis set for H, C, N and the LANL2DZ effective core pseudopotential for Pt. This calculation indicates a -0.21 partial charge on the alkynyl pyridyl nitrogens. Calculations to compare this ligand to 1,2-bis(2-pyridylethynyl)benzene and $Cp_2Ti(C_2$2py)$_2$, a previously reported metalloligand, are underway.

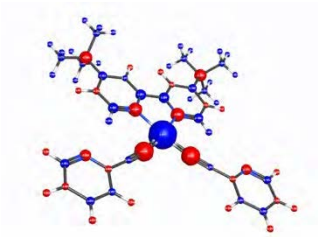


Figure 3: Electron Density Map of ^{t}BpyPt(C22py)$_2$

Regarding Cu (I) complexation, treatment of a CD_2Cl_2 solution of ^{t}bpyPt($C_2$2-py)$_2$ with $Cu(CH_3CN)_4PF_6$ afforded a new species (^{1}H-NMR). A single crystal of a Cu(I)-^{t}bpyPt($C_2$2-py)$_2$ complex was grown using the layering method with a DCM/Et_2O solution. X-ray analysis shows that the isolated single crystal is actually a dimer, [^{t}bpyPt($C_2$2-py)$_2$Cu]$_2$[PF_6]$_2$, with each Cu(I) atom η^2 bound to an alkyne on one Pt-molecule and a pyridyl ring on the other Pt-molecule. Similar multimodal binding of Cu(I) is seen in a Pt-cluster, [bpzPt($C_2$2py)2]$_2$[C_2py]$_2$$Cu_6I_2$ (where bzq = 7,8-benzoquinolinate). Here two of the Cu(I) atoms are η^2 bound to an alkyne and are also complexed to a pyridyl nitrogen. Regarding [^{t}bpyPt($C_2$2-py)$_2$Cu]$_2$[PF_6]$_2$, this compound is being formed during the crystal growth period and is not representative of the initial Cu(I) complexation. We are currently investigating the mechanism of this cluster formation.

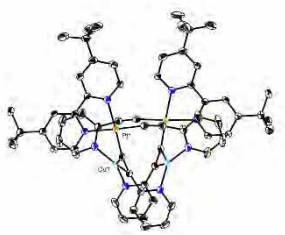


Figure 4: *[^{t}bpyPt($C_2$2-py)$_2$Cu]$_2$[PF_6]$_2$*

List of Objectives / Aims / Major Milestones Proposed	**Cumulative Outcomes / Accomplishments**
Train Students	8 students were trained during this project period, three students were trained as computational chemists, in addition to synthetic chemists.
Submit Proposal	An ACS PRF proposal was submitted. Although it wasn't accepted, the PI was asked to be a reviewer for these proposals and he plans on submitting a proposal this upcoming October.
Synthesize and characterize new ligands	The PI was successful in synthesizing ^{t}bpyPt($C_2$2-py)$_2$. This ligand was fully characterized including crystallographic data

	obtained from Clemson University. Interactions between this ligand and Pd(II) and Cu(I) salts were also characterized, with crystallographic data also obtained from Clemson University.
Establish an outreach Programs	Our group was able to establish outreach activities. Two outreach events were planned as a result of this grant, one involving a local private high school and the other involving a local group of home-schooled students.

Challenges & Strategies Used to Address / Overcome:
The PI struggled to get the computational resources running at full capacity. Although WebMo was successfully installed on the SimCenter's computer cluster, the program that it is interfacing with, GAMESS, is giving the PI issues with complex molecules. More of an effort could have been made to get GAMESS running, and other computational programs could have been investigated in more depth. The PI and his computational collaborator hope to continue working with members of the SimCenter to fix these issues.

The PI is dealing with this by training students on how to use these programs while the infrastructure is being set up. This way, when things are up and running, the PI will be able to make substantial research progress. The PI also is spending time with his students to generate input files that can be submitted as soon as things are running efficiently.

What didn't work? What did you disprove or learn from the parts that didn't meet your initial concept at the proposal?
The PI struggled to get the computational resources running at full capacity. Although WebMo was successfully installed on the SimCenter's computer cluster, the program that it is interfacing with GAMESS is giving the PI issues. More of an effort could have been made to get GAMESS running, and other computational programs could have been investigated in more depth. The PI and his computational collaborator hope to continue working with members of the SimCenter to fix these issues.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators
The PI was able to hire and train multiple undergraduate students because of this funding. (Funds like this that are able to pay for students are few and far between.) These students were able to help the PI set up his lab and also made significant research progress (a paper will be submitted this year). Moreover, two of these students were able to generate and run an outreach program using web-based computational chemistry. Because of this funding, the PI was introduced to Bailey Kirby, who has been an invaluable resource.

Students Impacted

Lara Partridge, who received fall 2018 and spring 2019 funding for research experience, biochemistry major, will attend medical school in the Fall of 2019.

Logan Jaques received fall 2018 funding for research and continued research for credit during the spring of 2019 and the summer of 2019 (funded by the chemistry department). Logan is a rising junior and a chemistry major, he plans to study natural products chemistry following his graduation.

Carson Gilbert received fall 2018 funding for research and continued research for credit during the spring of 2019 and the summer of 2019 (funded by the chemistry department). Carson is a rising junior and biochemistry major who plans on joining the military following college.

Hailey Beaver received spring 2019 funding for research. Hailey plans on attending medical school.

Sarah McDarmont received spring 2019 research for credit and summer 2019 funding and is a rising junior who plans on attending graduate school.

Anastasia McConkey, who received summer 2019 funding, is a rising senior who plans on attending pharmacy school.

Tiffany Truong received summer 2019 funding and is a rising sophomore who plans on attending graduate school.

Zach Moser received summer 2019 funding and is a rising senior who plans on getting a job in the chemical industry.

Community and Broder Impacts

We performed community outreach activities that center around browser based computational chemistry. Lara Partridge, and undergraduate researcher, developed three outreach activities that we shared with the surrounding community. One presentation was with a group of home-schooled students and the other presentation was with the members of GPS, a local private high school. Because of the one-time cost associated with the WebMO computational system, we will continue these types of activities following the funding period.

Scholarly Products

Publications:

1. N/A

External Conferences:

Five students are presenting at SERMACS in the fall of 2019.

Sarah McDarmont. Synthesis of multi-metallic acetylide compounds of d^{10} transition metal

Logan Jaques. Synthesis of ^{t}BpyPt($C_2$2py)$_2$ and its interactions with Cu(I) and Pd(II) metals

Zach Moser, Tiffany Truong, and Anastasia McConkey. Synthetic strategies for generating 4-ethynyl-2,3,5,6-tetrafluoropyridine

Presentations at UTC:

1. **J. Pienkos.** Research Dialogues.

Inventions or Other Intellectual Property
N/A

Research Outreach & Collaboration
The PI's students (Lara Partridge and Hailey Beaver) put on a computational workshop for students at GPS, a local private high school. The PI plans on working with Tracie Durham, the science chair at GPS, and one or two high school students during the Fall of 2019. Laura Partridge and Hailey Beaver also organized an outreach program with a group of home-schooled students in collaboration with Julie Bingham, a chemistry faculty member at UTC who commonly interfaces with these groups.

The PI and three of his students (Sarah McDarmont, Logan Jaques, and Carson Gilbert), put on a chemistry workshop for the honors college. During this workshop, the students and the PI covered chemistry techniques utilized in cooking (molecular gastronomy) and chemistry techniques utilized in purification (commonly utilized in the food industry). The synthetic training the students received during the period of the CSEACE grant allowed them to easily describe these purification techniques.

EXTERNAL FUNDING

Proposal Submissions
1. American Chemical Society, Petroleum Research Fund (ACS PRF) $55,000, not received)
2. Department of Energy-Early Career Funding Opportunity. NOI sent, and the PI was urged not to submit to this program.

Contracts/Awards Received
N/A

Sponsored Program Capacity Building Activities
1. NSF REU Workshop
2. NSF CAREER Workshop

WHAT'S NEXT FOR THIS RESEARCH?

How will you follow up your CEACSE grant with work in the next 1,2, … 5 years?
The PI will submit a publication in the next year describing research from this CEACSE grant. The PI will continue to provide outreach activities for the next few years. The PI will submit an ACS PRF grant this upcoming year to continually fund research related to this topic. The PI is acting as a reviewer for the ACS PRF committee. The PI will apply for an NSF grant and also apply for an NSF-care

What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?
The PI will submit an NSF grant this year, in collaboration with John Lee and Wang Yong Yang.

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?
The PI needs help with computer support. For the 2020 CSEACSE award, the PI would to have more organized meetings with the high-performance computing specialist. During these meetings, the PI will have his computational collaborator on hand and will discuss issues.

FINANCIAL ACCOUNTING

Remaining funds were based on a slight underestimation of supplies needed.

Fiscal Year 2019 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Mengjun Xie, Lead PI

Other Personnel:

PhD Student: Ruipeng Zhang, Department of Computer Science and Engineering

Project Title: “ULIRES: A Unified Live Incident Response System for Energy Delivery Systems”

Date Report Submitted: Aug. 26, 2019

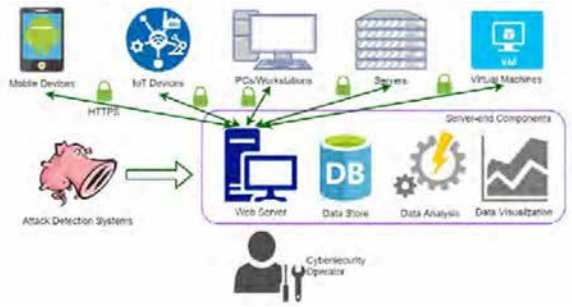
Award Start – End Date: August 15, 2018 – June 14, 2019

Non-Technical Summary:

As an indispensable component of a comprehensive cybersecurity solution to energy delivery systems, direct and efficient incident response has not received sufficient research and development efforts and therefore becomes a weak link. This project addresses the challenge of lacking in-depth research on effective technologies for forensics and incident response for energy delivery systems by developing ULIRES, a unified live incident response system. The core objective of this project is to develop a suite of novel, reliable, and efficient techniques that can be used to perform effective live incident response and to understand and model attack behavior for energy delivery systems. The research contributions include the design and development of new techniques for live system monitoring and data acquisition on an Android-powered mobile platform and IoT devices, as well as new knowledge of IoT incident response. The outcome of this research will result in transformative techniques that can lead to stronger security protection to the national energy infrastructure. This project will produce publications and software to the research communities and industry. This project has involved graduate students in the research, which advances the excellence in integrated and multidisciplinary research and education and aligns with the mission of SimCenter.

ULIRES: A Unified Live Incident Response System for Energy Delivery Systems

Technology Area of Interest: Cybersecurity, IoT

PROPOSED TECHNICAL APPROACH	OUTCOMES
• Design and development of unified, live data acquisition methods. • Design and development of data analytics and visualization methods. • Evaluation with an internal testbed through virtualization and simulation.	• Accurate, efficient, and systematic live forensic data acquisition mechanisms that can be controlled via user-friendly web GUI or CLI. • Secure communication, data exchange, and data store protocols. • Algorithms for analyzing and visualizing the forensic data. • Supervised data acquisition and forensic investigation.
RESULTS	**OTHER INFO**
 • We have implemented a prototype for remote live forensics for Android mobile devices, which serves as a base for ULIRES. • A manuscript is under preparation for a peer-reviewed venue.	**Budget and Schedule** Total Budget: $20,000.00 Actual Used: $20,000.00 Balance: $ 0.00 Total period of performance is 10 months. **Deliverables** • Final report detailing results, financials, and future work • Internal presentations • Software and documentation will be open source once the system is fully implemented and evaluated. **Organization Information** University of Tennessee at Chattanooga Computer Science & Engineering Mengjun Xie, Ph.D. Phone: (423) 425-5863 Email: mengjun-xie@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

In this project, we have developed GRRAndroid, a foundational component for ULIRES, a unified live incident response system for energy delivery systems. Figure 1 illustrates the general idea of ULIRES, which is designed on a client-server model. A software agent runs on every monitored client in an energy delivery system, which can be a smart mobile device, an IoT

device, a PC/workstation, a computer server, or even a virtual machine instance. Client agents securely communicate with the central server(s). The central server can be instructed by either human security operators or trustworthy external entities such as intrusion detection systems (IDS) to command specific client(s) to perform designated operations, upon an incident being detected. ULIRES provides much-needed data analytics and visualization functions to assist and facilitate live forensic investigation and incident response and assessment.

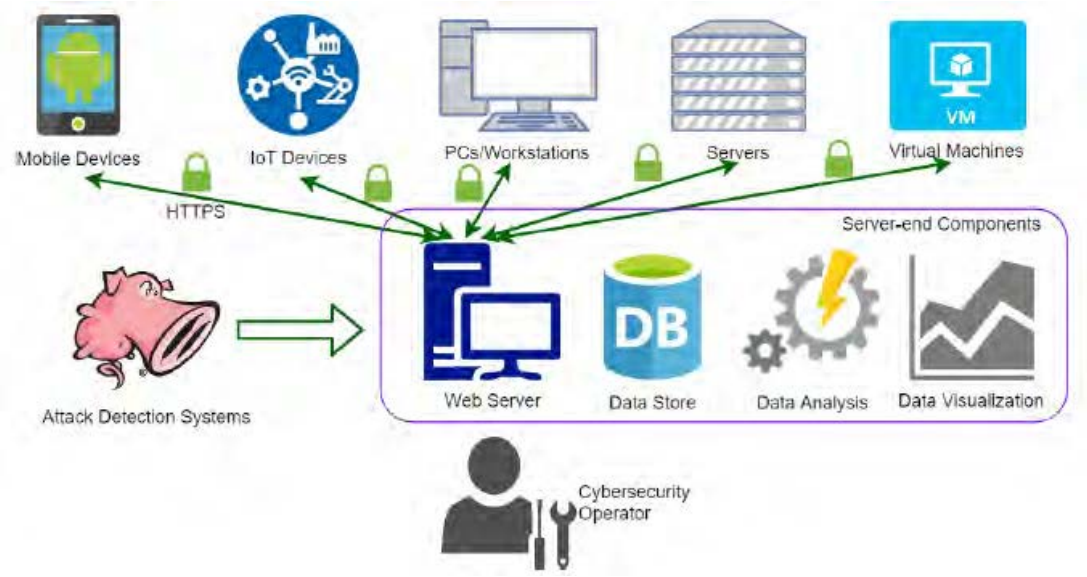


Figure 1. Overview of ULIRES System

We have developed a suite of novel, reliable, and efficient techniques that can be used to perform effective live incident response on Android platforms. GRRAndroid is able to:

1) Provide rapid, accurate, efficient, and systematic live forensic data acquisition mechanisms that can be fully controlled through a Web-based, user-friendly graphical user interface or command-line interface; All communications, data exchanges, and data stores are performed in a secure manner by applying standard-based security protocols and methods;
2) Monitor and interact securely and efficiently with a wide variety of devices: not only PCs and servers that run Windows, Linux, or Mac OS, but also Android mobile and IoT devices;
3) Assist cybersecurity operators in conducting interactive forensic data analytics and visualization and modeling attack behavior.

List of Objectives / Aims / Major Milestones Proposed	**Cumulative Outcomes / Accomplishments**
Develop data acquisition (client and server extensions for mobile and IoT devices), data analytics and visualization modules.	Live data acquisition modules including both client- and server-side modules for Android platforms; GRRAndroid prototype
Develop internal testbed, attack scenarios, and assessment criteria.	Design of assessment on GRRAndroid
Refine and improve data acquisition, analysis and visualization modules.	Documentation on GRRAndroid bug fixes and system improvement.
Conduct evaluation.	Preliminary evaluation on GRRAndroid.

THE UNIVERSITY OF TENNESSEE CHATTANOOGA
COLLEGE OF ENGINEERING AND COMPUTER SCIENCE

GRRAndroid: Remote Live Forensics for Android at Scale

Ruipeng Zhang, Mengjun Xie
Department of Computer Science
University of Tennessee at Chattanooga

RESEARCH DIALOGUES 2019

TECHNOLOGY SYMPOSIUM APRIL 18, 2019

Summary

GRRAndroid is a triage and logical data extraction tool for largescale remote live forensics of Android smartphones. It helps forensic investigators to collect digital evidence/artifacts in real-time from the investigated device without physical contact during the investigation. It can be easily integrated into custom Android firmware and access critical information without compromising the security of the underlying OS.

Motivation

- The smartphone market, as well as cybercrimes using or against smartphones, is skyrocketing and we need a better Android forensic tool
- Enterprise-scale mobility poses a higher scalability demand for cybercrime forensics
- Current Android forensic tools do not scale well and lack remote forensics functionalities

Challenges

- Supporting large-scale and in-time forensic triage and data acquisition. The system should be scaling-ready to keep up with the changing size of the device fleet and also consider network bandwidth usage.
- The comprehensive collection of evidence. Investigators can easily extract device information, sensor and user-generated data from Android devices of different OS versions without knowledge of the underline Android API.
- Minimizing performance impact on the system. The clients should have the minimum performance and energy impact on the Android device as the resources are open limited.
- Ensuring the integrity of the acquired evidence. A malicious party shall not disguise as either end of the system, nor can it steal or tamper with the evidence without knowing the keys of the client or the server.

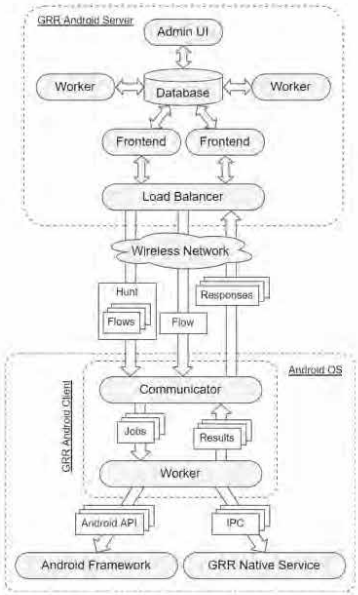
Project Description

Given the lack of efficient tools for large-scale mobile forensics and incident response, we propose GRRAndroid, a remote live forensic system that enables forensic triage and investigations for Android smartphones at scale.

In this project,

- We review the existing forensic tools for Android devices and present GRRAndroid.
- We evaluate the system comprehensively and present detailed result interpretation.
- We discuss the applications of GRRAndroid and how can it be integrated with other systems to reinforce the enterprise mobile environment.

System Design



Results

Supported Data Types

- Device and system information
- Contacts/Address book
- Installed Apps
- Call history/Call log
- Storage information
- Short messages (SMS & MMS)
- Battery status
- System settings
- Cellular and telephony information
- Sensor information and data (Gravity, Accelerometer, etc)
- WiFi access points and connection information
- Localization and timezone settings
- Bluetooth information
- NFC information
- GPS/Geolocation information
- User accounts*
- System users*
- VPN settings*
- Filesystem*
- Network connections*
- Running processes*
- Web browsing history*
- Lock screen/Fingerprint key file*

* In system privileged app mode

We also evaluate GRRAndroid in the following aspects:
♦ Scalability ♦ Energy Consumption ♦ Robustness ♦ Security

Discussion

- Our solution is suitable for cooperatives that adopt the corporate-owned-personally-enabled (COPE) mobile management model.
- Our mobile clients can work well under both system-privileged-app mode and normal mode, no device rooting is required.

References

Ruipeng Zhang, Mengjun Xie, "GRRAndroid: Remote Live Forensics for Android at Scale", unpublished.

Challenges & Strategies Used to Address / Overcome:

It is much more difficult than expected to integrate our Android live forensic framework with an existing industrial-level system (Google GRR) than doing a fresh implementation because of its massive codebase and lack of documentation.

The evaluation of our Android forensics system requires user interaction, which is difficult to predict and time-consuming. We circumvented that problem using automated UI testing provided by Android SDK.

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 the time and budget limitation of this project, we were not able to implement a smart grid testbed and test our system. We will continue our investigation in the future.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This project allows the PI to initiate a new research topic and integrate his research experiences and skills in cybersecurity, networking, and Internet of Things. It also opens an opportunity for him to collaborate with other researchers at UTC regarding Smart City and IoT security.

Students Impacted

Mr. Ruipeng Zhang,a Ph.D. student in Computer Science. He has been working on this project for the past year. With the research funds from CEACSE, he was able to continue his study and pursue a Ph.D. degree. He has acquired valuable hands-on research experience and knowledge of digital forensics and research project management through this project.

Community and Broader Impacts

The outcome of this research can make significant broader impacts on the nation's energy delivery systems. This project has laid a solid foundation for development of transformative techniques that can lead to stronger security protection to the national energy infrastructure. The research outcome will be incorporated into both undergraduate-level and graduate-level security courses offered at UTC. Moreover, the PI will host seminars on this research topic, sponsor senior projects, and present the research outcome to local K-12 and community college students to attract more students into STEM disciplines.

Scholarly Products

Publications:

Ruipeng Zhang and **Mengjun Xie**. “GRRAndroid: Remote Live Forensics for Android at Scale.” Under preparation for submission.

Presentations at UTC:

M. Xie. ReSEARCH Dialogues, 2019.

M. Xie. CECS Technology Symposium, 2019.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

1. Decentralized and Secure Remote Control for Internet of Things, submitted to CEACSE Grants Competition FY 2020, Amount: $98,706, Status: declined.

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. Ruipeng Zhang attended IEEE ICC 2019 conference and presented our paper on cloud computing security with partial support from this grant.

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 system development and evaluation of ULIRES. We also plan to expand the ULIRES to other IoT scenarios and apply data mining and deep learning techniques to analyze collected data. By doing so, we can have a deeper understanding of the cyberattacks against IoT systems. Our preliminary findings and outcome of this project will be used in ULIRES’s future development and contribute to grant applications.

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

Our future research focus will also include cloud network intrusion detection and blockchain-based IoT security.

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: $20,000.00

Cumulative Expenditures: $20,000.00

Remaining Award Amount: $0.00