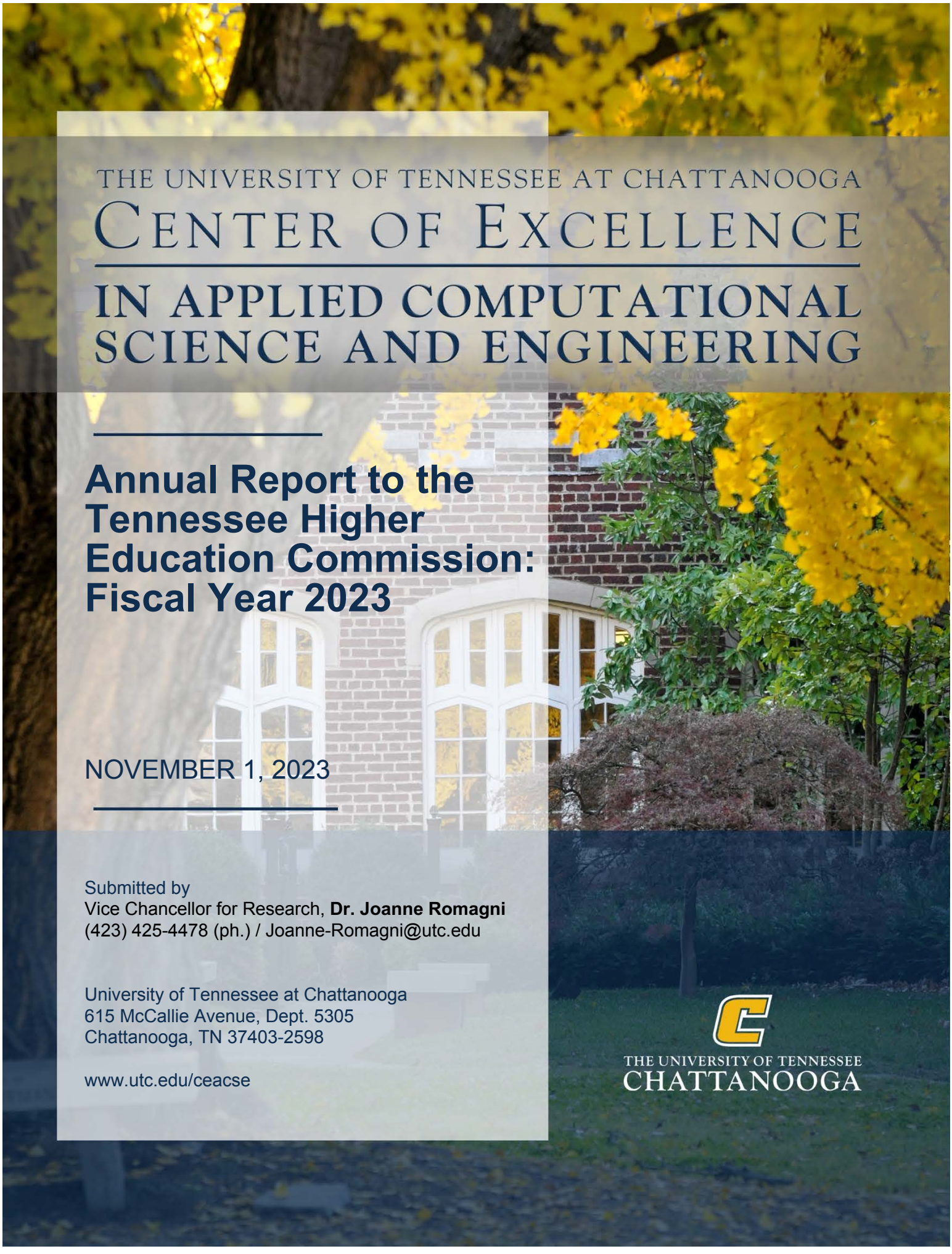

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

Annual Report to the Tennessee Higher Education Commission: Fiscal Year 2023

NOVEMBER 1, 2023

Submitted by
Vice Chancellor for Research, **Dr. Joanne Romagni**
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THE UNIVERSITY OF TENNESSEE
CHATTANOOGA

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 through mentoring of students and faculty, seed funding in key thrust areas, and providing state-of-the-art research computing facilities.

VISION STATEMENT

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

EXECUTIVE SUMMARY

The University of Tennessee at Chattanooga's (UTC) Center of Excellence in Applied Computational Science and Engineering (CEACSE), which we call SimCenter for short, continues has completed its second decade in 2023 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. We look to a future of continued excellence as we begin our 22nd year in Fall 2023.

With our previous report for FY2022, CEACSE marked its 20th 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 FY2023 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 a variety of 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. Significantly, the number of industrial and national lab internships and full-time jobs landed by graduating SimCenter students is growing. The continued success of prior CEACSE-funded professors in growing their science and engineering inquiries, and external funding, is also notable.

Some notable outcomes in FY2023 include these highlights:

- PI Yang's Ph.D. student successfully defended his dissertation
- PI Gao's graduate student assistant was accepted into a Ph.D. program at Purdue University
- PI Affare participated in a National Science Foundation (NSF) Panel
- PI Alda-Pons' research resulted in the completion of a master's thesis in the department of Biology, Geology, and Environmental Science and established a new researching line at UTC about metabarcoding and the gut microbiome
- PI Alda-Pons' research was published in *Biochemistry and Biophysics Report* and *Biomolecules* and was presented at Vanderbilt's Undergraduate Research Fair, the Association of Southeastern Biologists Annual Meeting in both 2022 and 2023

- PI Ibrahim's project was presented in the International Conference on Metallurgical Coatings and Thin Films and the 14th Symposium on Biodegradable Metal for Biomedical Applications
- PI Manning-Berg's project was presented at the Southeastern-Northcentral Geological Society Meeting and the National Geographic Society Meeting
- PI Ranjan's project resulted in three software products: MINCLES, UTCFOAM, and OS-Solver
- PI Yang received outside funding from both FLY Competition and OCSD
- PI Smith developed FEniCS code as a part of his project

Also, from CEACSE funds for FY2023, we awarded five core awards (maximum of $100,000) and three Initiation/Opportunity Awards ($15,000 each).

In collaboration, the 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 maturing in its role at UTC as a nexus of research incubation, HPC and data science, and as a key provider of faculty resources that complement and supplement ORSP's offerings and those of faculty home departments.

This document constitutes the Annual Report for Fiscal Year 2023 of CEACSE activities and efforts. On behalf of UTC, SimCenter, our community partners and stakeholders, and our CEACSE-funded scientists, engineers, and students, we express our deep appreciation to THEC for this critically important support of the CEACSE at the University of Tennessee at Chattanooga.

Schedule 7, included on page 19, details our FY2023 budget and expenditures for FY2023, as well as outyear requests.

TABLE OF CONTENTS

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 for this reporting period was Dr. Tony Skjellum. 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 FY2023 Awardees

The following faculty and staff were integral to the strategic direction of CEACSE during the 2022–2024 competition cycle, on both core and Faculty Initiation/Opportunity Awards. As noted below, these individuals served as a Lead PI and/or Co-PI on projects that advanced the CEACSE mission and vision. Biosketches for all faculty may be found in **Appendix A**.

Dr. Sandra Affare

Dr. Sandra C. Affare is a retired TVA engineer and current UTC engineering professor, who often bridges the gap between academia and the business sector. Dr. Affare is an advocate for women in engineering and other underrepresented roles, including leadership. For this project, Dr. Affare will rely heavily on her 16 years of project management professional experience and will co-lead the curriculum development corhort, coordinate the team of collaborators, and co-manage the project. She will also assist the participants in applying the Scientific Method while researching food insecurities in the community.

Lead PI: "Food Desert Identification and Elimination System"

Dr. Murat Barisik

Dr. Murat Barisik is currently an assistant professor in Mechanical Engineering at UTC. He received his Ph.D. in Aerospace, Aeronautical and Astronautical Engineering from Old Dominion University in 2012. Dr. Barisik's academic and professional career has centered on integrating mechanical engineering and computational theories and techniques for molecular-level investigation of the nano-scale transport phenomena. The span of his research shows a diverse level of expertise in the nano-technology-related areas including nano-scale gas transport, nano-scale heat transfer and nano-scale electrokinetic phenomena. He is the author of 3 book chapters and 45 scientific papers in international journals which received over 1700 citations. Recently, he received support from the Department of Energy to investigate reactive gas flows collaborating with Oak Ridge National Laboratories.

Lead PI: "Molecular modeling of electric double layer and nanoscale heat transfer in supercapacitors"

Dr. Tian Li

Dr. Li joined UTC in August, 2022 as an Assistant Professor of Physics. Dr. Li received his Ph.D. in Physics in Dec. 2017 from the Joint Quantum Institute (JQI), National Institute of Standards and Technology (NIST) and the University of Maryland, College Park.

Prior to UTC, Dr. Li was an Associate Research Scientist (promoted from a Postdoctoral Research Associate) in the Institute for Quantum Science and Engineering and the Department of Biological & Agricultural Engineering at Texas A&M University.

Dr. Li specializes primarily in experimental quantum optics. He uses atomic vapor as well as nonlinear optical crystals to generate quantum correlations and entanglement for quantum information, quantum sensing and quantum imaging investigations. Dr. Li is a key member of the UTC Quantum Initiative and is leading the effort to build a Quantum Node Lab which provides the access to the EPB Quantum Network - the first commercial quantum network in the world. When he's not in his office or labs assisting students with advancing the frontiers of quantum optics, he's either learning to master acoustic guitar or messing around with his kid.

Lead PI: "Towards Quantum Enhanced Bio-Sensing"

Dr. Fernando Alda

Dr. Alda is an evolutionary biologist with a broad interest in understanding the mechanisms that generate biological diversity, and particularly in the relative roles of geological and ecological factors driving within and among species variation. His research focuses on patterns and processes controlling the evolution and diversity of—mostly but not only—freshwater fishes, which he studies using a combination of fieldwork, phylogenomic systematics, population genetics and collections-based research tools that allow him to reach broad goals in ecology and evolution including: biogeography, speciation, and conservation.

Co-Investigator: "Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome"

Dr. Yu Liang

Dr. Yu Liang is currently working at the Department of Computer Science and Engineering of University of Tennessee at Chattanooga as a Full Professor. His funded research projects cover the following areas: big-data and cloud computing, modeling and simulation, machine learning and artificial intelligence, high-performance scientific, numerical linear algebra, sensor and actuator, biomedical engineering, and computational mechanics. His research work has appeared in various prestigious journals, book or book chapters, and refereed conference, workshop, and symposium proceedings. Dr. Liang is serving in the Data (https://www.mdpi.com/journal/data) , 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.

Lead PI: "Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome"

Dr. David Giles

Microbial survival is dependent upon adaptation to the surrounding environment. Dr. Giles is interested in those responses occurring in microbial membranes that involve conserved microbial structures, such as phospholipids and lipid A. These membrane constituents can be modified in a variety of ways depending upon external environmental stimuli or simply by nutrient availability. Lipids of various types and origins can be encountered by microbes and used as signaling molecules, membrane building blocks, or energy sources. Projects in Dr. Giles' laboratory currently involve surveying the lipid content of several bacteria of medical importance in response to environmental and host-specific conditions. He is also interested in extending his research towards aquatic microorganisms of medical and ecological importance.

Lead PI: "From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes"

Dr. Steven Symes

Dr. Steven Symes has been a member of the faculty at UTC since 1999.

Dr. Symes earned his Bachelor of Arts degree in Physics in 1992 at Washington University and his Ph.D. in 1996 at the University of Arkansas. He was a Post-doctoral Fellow from 1996 to 1998 at the NASA Johnson Space Center in Houston, TX.

His professional interests include analytical chemistry, quantitative analysis of the major and trace-element chemistry of planetary materials.

Co-Investigator: "From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes"

Dr. Bradley Harris

Dr. Bradley Harris is an Assistant Professor in the Civil and Chemical Engineering Department at the University of Tennessee at Chattanooga (UTC). He received his PhD (2014) in Chemical and Biomolecular Engineering at the University of Tennessee Knoxville. 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: 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 disease pathogenesis, environmental remediation, and renewable energy. 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 high school and community college students and local industry professionals in chemical engineering through the development of a remote laboratory. He 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 (IoT).

Co-Investigator: “From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes”

Dr. Hamdy Ibrahim

Dr. Ibrahim is an Assistant Professor in the Mechanical Engineering Department at the University of Tennessee at Chattanooga. Before joining UTC, he worked as a postdoctoral fellow in the dynamics and smart systems lab (DSSL) at the University of Toledo, Ohio. He also worked as a Chief Research Officer for the start-up company Thermomorph, LLC aims to develop Nitinol-based biomedical devices. In this capacity, he participated in several NSF funded programs, such as the National I-Corps and the Small Business Innovation Research (SBIR). Dr. Ibrahim completed his Ph.D. in Mechanical Engineering from the University of Toledo in August 2017. He also completed his M.Sc. in May 2012 after obtaining a B.Sc. Hons Degree in May 2008, both in Mechanical Engineering, from Cairo University. Dr. Ibrahim’s research findings on biomaterials have resulted in 2 patent applications and over 20 peer-reviewed journal and conference publications. His research interests include biodegradable metals, biocomposites, shape memory alloys, additive manufacturing, surface treatments, and corrosion behavior of biomaterials

Lead PI: “Topological design of porous metals for biomedical applications” and” Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants”

Co-Investigator: “Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials”

Dr. Eleni Panagiotou

Dr. Panagiotou's research in interdisciplinary and also spans pure, applied and computational mathematics. In particular, she is interested in the effects of topological entanglement in physical systems, such as polymers. The study of topological entanglement in polymers involves the creation of new topological/ geometrical tools for such systems and their application to physical systems through molecular simulation. Dr Panagiotou obtained her PhD at the National Technical University of Athens, Greece, on Applied Mathematics. She has had visiting research positions (funded) at the ETH Zurich, Switzerland (Department of Materials) and the Newton Institute for Mathematical Sciences in Cambridge, UK. She was a Visiting Assistant Professor and Visiting Lecturer at the Department of Mathematics at the University of California Santa Barbara before coming to UTC. In UTC, she was awarded and NSF RUI grant for research on Topological methods for studying polymer entanglement.

Co-Investigator: “Topological design of porous metals for biomedical applications”

Dr. Mohamad Mahtabi

Dr. Mohammad Mahtabi received his PhD in Mechanical Engineering from Mississippi State University and was a post-doctoral researcher for about a year at The University of Toledo, before joining the Mechanical Engineering Department at UTC. Dr. Mahtabi holds a bachelor’s degree from The University of Tehran and a master’s degree from Iran University of Science and Technology. He has also worked for about seven years in the industry as a structural engineer. Dr. Mahtabi’s research area includes experimental and

computational aspects of additive manufacturing (a.k.a. 3D printing), fatigue and fracture mechanics, mechanical behavior of materials and shape memory alloys.

Lead PI: "Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials"

Co-Investigator: "Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants"

Dr. Daniel Loveless

Dr. Daniel Loveless is a UC Foundation Associate Professor of Electrical Engineering at UTC. He received a B.S. degree in electrical engineering from Georgia Institute of Technology, Atlanta, Georgia, in 2004 and M.S. and Ph.D. degrees in electrical engineering from Vanderbilt University, Nashville, Tennessee, in 2007 and 2009, respectively. Prior to joining UTC in 2014, Dr. Loveless was a senior engineer and Research Assistant Professor at the Institute for Space and Defense Electronics (ISDE) at Vanderbilt University. 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; and CubeSat design. Dr. Loveless has published approximately 100 articles in peer-reviewed journals and is a Senior Member of IEEE. He currently serves as an Associate Editor of the IEEE Transactions on Nuclear Science. His honors include the inaugural 2019 Nuclear and Plasma Sciences Society (NPSS) Radiation Effects Early Achievement Award, five best conference paper awards, and the IEEE NPSS Graduate Scholarship Award for recognition of contributions to the fields of nuclear and plasma sciences.

Co-Investigator: "Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)"

Dr. Donald Reising

Dr. Donald R. Reising is a Guerry and UC Foundation Associate Professor of Electrical Engineering at the University of Tennessee at Chattanooga (UTC). Dr. Reising received a B.S. degree in electrical engineering from the University of Cincinnati, Cincinnati, Ohio, in 2006 and M.S. and Ph.D. degrees in electrical engineering from the Air Force Institute of Technology (AFIT), Wright-Patterson Air Force Base (WPAFB), Ohio, in 2009 and 2012, respectively. Before joining UTC's faculty in 2014, Dr. Reising served as an electronics engineer and researcher at the U.S. Air Forces Aeronautical System Center (2006 – 2009) and Research Laboratory (AFRL) Sensors Directorate (2009 – 2014). His research interests include digital communications and signal processing; Specific Emitter Identification (SEI) and Radio Frequency (RF) fingerprinting; next generations communications systems; automation of smart grid electrical disturbance categorization, identification, and learning; as well as the use of SEI, machine learning, and signal processing in radiation effects characterization. Dr. Reising is a member of Eta Kappa Nu, Tau Beta Pi, and a Senior Member of IEEE. His honors include IEEE Chattanooga Chapter's Outstanding Engineer Award (2022), UTC's Outstanding University Service Award (2018), AFRL Sensors Directorate Dr. Samuel M. Burka Award (2013), Association of Old Crows Research Excellence Award (2009), and the Measurement and Signature Intelligence (MASINT) Committee Academic Excellence Award (2009).

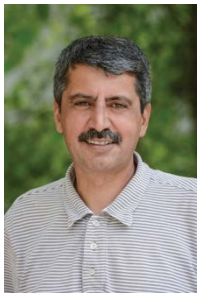
Lead PI: "Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)"

Dr. Ashley Manning-Berg

Dr. Manning-Berg's research involves using chemical sedimentary rocks to investigate the geochemical composition of Earth surface environments and the effects of early diagenesis in these systems. Most of her research has focused in the Precambrian, and the geochemical conditions of marginal marine environments and early Earth. Such geologic settings aid in the understanding of early life on Earth and provide analogs for potential extraterrestrial microbial life.

Lead PI: "Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record"

Dr. Abi Arabshahi



Dr. Abi Arabshahi is a former 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.

Co-Investigator: "Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record"

"Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites"

Dr. Hong Qin

Dr. Hong Qin is a Professor and Head of 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.

Lead PI: "Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2"

Dr. Ziwei Ma

Dr. Ma is an assistant professor of statistics in Department of Mathematics at University of Tennessee at Chattanooga (UTC). He received his Ph.D. in Mathematics (specialized in Statistics) from New Mexico State University at Las Cruces, NM. His research involves in mathematical and applied statistics and machine learning.

Co-Investigator: "Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2" and "Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy"

Dr. Azad Hossain

Azad Hossain is an expert in digital image processing, remote sensing, GIS, and spatial analysis. Technical skills include but not limited to: GIS data creation and editing, GIS data management and analysis, Geo-spatial modeling (graphical modeling), Image Processing and analysis with optical (multispectral and hyperspectral data) and microwave data, Decision Support Systems (DSS) Design and Geostatistical Analysis.

He has more than 15 years of experience in different GIS and digital image processing softwares such as ArcGIS (PC Arc Info, Arc Info Workstation, ArcServer), ERDAS Imagine and ENVI. Has professional trainings on ESRI PC Arc/Info 3.4, ArcView GIS 3.1, ArcView Spatial Analyst 2.0, Arc/Info 8.02, ArcIMS, Trimble GPS/DGPS, CalComp Plotter, Microsoft Access and Visual Basic.

Dr Hossain has working experienced in 2D and 3D numerical models for simulating flow, sediment transport and water quality, Visual Basic Application, Arc Objects, Python and Fortran programing languages.

Dr. Hossain's research insterests include application of GIS, remote sensing, and spatial analysis in different areas of earth and environmental science. He is specifically interested in 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.

Current Research Focus: Urbanization, surface water quality, landslides, and sinkholes in Chattanooga, TN. Geospatial Big Data.

Co-Investigator: "Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2"

Dr. Reetesh Ranjan

Dr. Reetesh Ranjan is an Assistant Professor in the Department of Mechanical Engineering at the University of Tennessee at Chattanooga. He received M.S. and Ph.D. in Theoretical and Applied Mechanics in 2009 and 2012, respectively, from the University of Illinois at Urbana-Champaign, and B. Tech. in Mechanical Engineering from the Indian Institute of Technology Kanpur in 2004. He worked at Ansys India from 2004 to 2007 as a Lead Application Engineer. He worked in the School of Aerospace Engineering at Georgia Institute of Technology from 2013 to 2019 as a Post-Doctoral Fellow, Research Engineer, and Senior Research Engineer. He has received Fred B. Seely and Louis J. Larson fellowships, and Hassan Aref Memorial award for his academic and research accomplishments during his graduate education. He has also received Stanley I. Weiss

outstanding thesis award in 2013 from the Department of Mechanical Science and Engineering at the University of Illinois at Urbana-Champaign for his Ph.D. dissertation.

Lead PI: "Modeling of Transition to Turbulence in Large Eddy Simulation using the Two Level Simulation Approach"

"Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy"

Dr. Sungwoo Yang

Dr. Sungwoo Yang, an assistant professor, joined in the Civil and Chemical Engineering Department at the University of Tennessee at Chattanooga (UTC) in the Fall of 2017. He received his PhD (2011) at Duke University, then joined MIT as a postdoctoral fellow to conduct research within the Device Research Laboratory (with Prof. Evelyn Wang). Later, he became a research scientist at MIT in 2014.

Lead PI: "A Low-Cost, Passive Solar Process Heat System" and"Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss"

Dr. Morgan Smith

Dr. Smith received his PhD in Anthropology from Texas A&M University, where he studied in the Center for the Study of the First Americans. Prior to this, he worked for the Southeast Archaeological Center of the National Park Service in the section 106 compliance division. Dr. Smith has over a decade of experience in underwater and terrestrial archaeology and has directed multiple full-scale geoarchaeological excavations of underwater prehistoric sites as well as Phase I and Phase II surveys of terrestrial and submerged lands throughout North America. His contributions to underwater archaeology include efforts to develop methods and models to more accurately and reliably locate underwater prehistoric sites, with an emphasis on mobile forager societies. He has conducted archaeological and anthropological research in Florida, Georgia, Alabama, North Carolina, Mississippi, Tennessee, Missouri, Texas, Nevada, Mexico and Costa Rica.

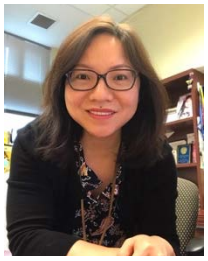
Lead PI: "Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites"

Dr. Boris Belinskiy

Dr. Belinskiy was born in 1946 in St. Petersburg, former Soviet Union. He graduated with an MS in Math Physics from St. Petersburg (Leningrad) St. Univ. in 1970 and his PhD. In 1972. He received his D.Sc. from same in 1986. He emigrated to the USA in 1991 and was employed at Univ. of North Florida before coming to UTC where he received a UC Foundation professorship in 1996.He is a current member of the Council of Scholars.

Co-Investigator: "Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites"

Dr. Lani Gao



Dr. Lani Gao is currently a professor in statistics at UTC and biostatistician at University of Tennessee College of Medicine at Chattanooga. Her primary research includes genetics/genomics data analysis, statistical/machine learning for complex data, high-dimensional data analysis, and data science challenges. She applies her expertise to big data analytics in engineering, neuroimaging, epidemiology, and biomedical science. Recently, she focuses on time series forecasting using social media data like Google Trends and developing statistical methods to validate AI-based healthcare tools. Her contributions span various domains, showcasing a commitment to advancing data-driven insights and applications.

Lead PI: "Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy"

Dr. Nagwan Zahry

Dr. Zahry is an Assistant Professor in the Department of Communication. She received her PhD in Media & Information from Michigan State University in the fall of 2017. During her PhD at the Michigan State University's College of Communication Arts and Sciences, she worked in many interdisciplinary projects implemented by the College of Nursing, the College of Engineering, and the College Agriculture and Natural Resources.

Prior to joining UTC in 2012, Dr. Zahry worked as a Assistant Professor at Michigan State University's Department of Public Relations and Advertising where she taught undergraduate and graduate courses.

Co-Investigator: "Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy"

FY2023 STUDENTS

Project Title: “Food Desert Identification and Elimination System”
Lead PI: Sandra Affare

Students Impacted:

Dexter Digby: Mr. Digby is a Senior Engineering Management and Technology undergraduate student who is scheduled to graduate in December 2023. The student worked on the project during the Fall 2022 semester and received an internship with the Electric Power Board beginning in the Spring of 2023. During the Mid Term Status meeting, Mr. Digby presented a working prototype of the web-based tool that will be used to collect data and document food access and food security concerns.

Markintus Morris: Mr. Morris is a Computer Science and Engineering Management undergraduate student. He worked on the project for less than two months in the Spring of 2023.

Project Title: Molecular modeling of electric double layer and nanoscale heat transfer in supercapacitors
Lead PI: Murat Barisik

Students Impacted:

NA

Project Title: Towards Quantum Enhanced Bio-Sensing
Lead PI: Tian Li

Students Impacted:

Matthew Boone, a physics sophomore, has successfully completed his summer URP under the supervision of the PI focusing on improving the communication rate of BB84 quantum key distribution algorithm. The results of this investigation will be presented in the 90th Annual Meeting of Southeastern Section of the American Physical Society, which will be held in Eastern Kentucky University from Nov. 9th to Nov. 11th.

Project Title: Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome
Lead PI: Fernando Alda

Students Impacted:

The student, William Hanson-Regan was funded by this project, learned field work, molecular, and computational skills, presented his work at a local conference, and is currently in a scientific manuscript. Two undergraduate students were also funded by this project and an additional undergraduate student obtained undergraduate research credits working in this project.

William Hanson-Regan: Graduate student in the Environmental Science Program at the University of Tennessee at Chattanooga. Defended his M.Sc. Thesis in August 2023 based on the current project.

Breann Larson: Undergraduate student in Environmental Science at the University of Tennessee at Chattanooga. Was a summer student worker in this project carrying out fieldwork activities and assisting graduate student William Hanson-Regan in this project.

Joseph Watson: Undergraduate student in Biological Science at the University of Tennessee at Chattanooga. Was a summer student worker in this project carrying out fieldwork, and molecular laboratory activities to assist graduate student William Hanson-Regan in this project.

Sebastian Jimenez: Undergraduate student in Biological Science at the University of Tennessee at Chattanooga. Assisted graduate student William Hanson-Regan in this project carrying out molecular laboratory activities.

Project Title: From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes
Lead PI: David Giles

Students Impacted:

Andrew Turgeson, Ph.D. student, Department of Chemical Engineering: first author on publication; generation of data for future manuscripts; excellent experience for his post-doc application.

Naina Patel, undergraduate student, Department of Biology, Geology and Env. Science: received support from the grant as she performed experiments for her departmental honors project. Naina will graduate in December and her data has been presented at a research conference and will be preliminary data in a grant application.

Benjamin House, undergraduate student, Department of Chemistry and Physics: Ben spearheaded the preparative TLC and UPLC/MS studies during the summer of 2022. He continues to be compensated from the grant and is working on analysis of data. Because of the CEACSE, Ben began working on another project in my laboratory and saw it to completion, earning authorship and padding his application for medical school (accepted to Vanderbilt).

Saksham Saksena, undergraduate student, Vanderbilt University: Saksham was my REU student during the summer of 2022. He was able to interact with students and myself working on the CEACSE, which undoubtedly benefitted his perspective on his own bioinformatic project which was published during the funding period.

Lucas Morley, undergraduate student, University of Pittsburgh: Andrew Turgeson (and Dr. Harris) trained Lucas (an REU student) on how to generate molecular models of membranes and associated simulations. His training was enriched due to the CEACSE-related data and opportunities.

Olivia Chester, undergraduate student, UTC: Olivia gained training during the project and made contributions to the data on this grant as well as another collaborative project.

Meredith Grant, undergraduate student, UTC: Meredith was trained and has become an expert at performing MIC assay, many of which pertained to this project.

Mallory Anderson, undergraduate student, UTC: Mallory also gained experience and learned MIC assays that informed the project. She graduated May 2023 and was trying to gain employment in Germany.

Project Title: Topological design of porous metals for biomedical applications
Lead PI: Hamdy Ibrahim

Students Impacted:

Hemanth Kumar, Masters student: Worked on the project and was fully funded. Student in the Math Department at UTC.

Rahul Kshatri, Masters student: Worked on the project and was partially funded from the project for one semester. Student in the Mechanical Engineering Department at UTC.

Vipul Patil, Masters student: Worked on the project and was partially funded from the project for two semesters. Student in the Mechanical Engineering Department at UTC.

Gage Plotner, Undergraduate student: Worked in the project and was partially funded for one semester.

Project Title: Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants
Lead PI: Hamdy Ibrahim

Students Impacted:

Ahmed Korra, Masters student: He was partially funded. He graduated in Summer 2023.

Shelby Hash, Undergraduate student: She was partially funded in this project during Fall 2021 and Spring 2022.

Andre Flores, Undergraduate student: He was partially funded in this project during Fall 2022 and Spring 2023.

Adrianne Glover, Undergraduate student: She was partially funded in this project during Spring 2023 and Summer 2023.

Joshua Rich, Undergraduate student: He was partially funded in this project during Spring 2023 and Summer 2023.

Project Title: Anti-Tamper IC Forensics and RF-Level DIscrimiNation For Improved Trust (INFORM)
Lead PI: Daniel Loveless

Students Impacted:

Jake Carpenter (GA), Berkay Dean (UG), Trevor Peyton (UG)

Project Title: Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials
Lead PI: Mohamad Mahtabi

Students Impacted:

Saeed Ataollahi (PhD student, conducted the computational work and calibrating the potentials - expected graduation Dec. 2023) worked on this research. The results of this work will form a large portion of his PhD dissertation. So far in this project, he has co-authored two conference papers, two journal articles, and will be submitting two more journal articles.

Mitchell Bauer (UG student): involved in research activities. Learned about the science of materials, shape memory alloys (SMAs), and their processing. He has become very interested in research on materials and is seriously considering post-graduate studies.

Project Title: Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record
Lead PI: Ashley Manning-Berg

Students Impacted:

Elizabeth (Katee) Lam (seeking a B.S. in History) – Katee has growing microbial consortiums mats and monitoring decomposition. From this experience she has learned how to use the microscope and basic laboratory skills. She has presented her research at Research Dialogues and has been a co-author one 3 Geological Society of America (GSA) presentations- two national and one regional (funding limitations and class conflicts prevented her presenting at the conferences).

Matthew (Gage) Plott (just finished M.S. in Math) - Gage worked with the R code over the summer of 2022. He was able to compare the parameters listed in the published papers to the associated code and annotate the code for me. He also helped me to identify areas where changes to the code may be beneficial(e.g., atmospheric concentrations for oxygen and CO2, and time steps for organism death within the modeled microbial mat). He also deciphered the biomass concentrations for several days after the initial spin-up of the model. The data provided a biomass value every 12 hours that might be able to be used for a starting biomass in other models.

Project Title: Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2
Lead PI: Hong Qin

Students Impacted:

Landen Bauder, MS student

Connor Firat, MS student

Parisa Hatami, Ph.D. student

Gertrude Osei, MS student

Braxton Anzalone, BS student.

Project Title: Modeling of Transition to Turbulence in Large Eddy Simulation using the Two Level Simulation Approach
Lead PI: Reetesh Ranjan

Students Impacted:

Mickael Young (MS with thesis option, Fall 2022)**:** Mr. Young learned to carry out high-fidelity turbulent flow simulations using HPC resources. Additionally, he learned the skills to analyze large-scale datasets generated from simulations using Python. He also implemented a MATLAB-based solver for the Orr-Sommerfeld equations, which was key to the research project. His key focus was to carry out simulations of transitional flows and analyze statistical, structural, and spectral aspects of such flows. He has been trained in the usage of tools such as TLSLES solver, Tecplot, Paraview, Python, GitHub, Latex, Trac, and Cantera. He has contributed to two conference presentations, one conference article, one poster, and one UTC conference.

Eli Durant (MS, expected graduation Fall 2023)**:** Mr. Durant has learned several skills ranging from pre- to post-processing and running the simulations using HPC resources provided by SimCenter. He has learned tools such as Python, UTCFOAM, Tecplot, Paraview, Pointwise, Trac, etc. He has been trained in understanding the physics of wall-bounded turbulent flows. He has contributed to a conference presentation, a conference article, a poster, and a UTC conference.

Robert Smith (Undergraduate, graduated Fall 2022): Mr. Smith has learned to run the simulations using HPC resources provided by SimCenter. He has also learned tools such as Python, UTCFOAM, Tecplot, Paraview, Pointwise, Trac, etc. He has been trained specifically on mesh generation and post-processing of simulation results. He has contributed to a conference presentation, a poster, and a UTC conference.

Project Title: Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy
Lead PI: Reetesh Ranjan

Students Impacted:

Steven Thompson (MS with thesis option, Expected Graduation in Summer 2024)**:** Mr. Thompson learned to carry out high-fidelity simulations of stratified turbulence using HPC resources. Additionally, he learned the skills to analyze large-scale datasets generated from simulations using Python. A key focus was to analyze statistical, structural, spectral, and modal aspects of stratified turbulence. He has been trained in the usage of tools such as MINCLES solver, Tecplot, Paraview, Python, GitHub, Latex, Trac, and POD/DMD tools. He worked on this project in Fall 2022 as an undergraduate researcher before switching to MS in Spring 2023.

Amin Amiri (MS, Expected Graduation in Summer 2024)**:** Mr. Amiri was trained to carry out high-fidelity simulation using HPC resources. He implemented data-driven based pre-processing scripts using TensorFlow software and LES model relying on deep neural network for simulation of wall-bounded turbulent flows.

Robert Smith (MS, Expected Graduation in Summer 2024): Mr. Smith has worked on implementing modules for performing simulation of forced isotropic turbulence.

Nelson Rainey (UG, Graduated in Fall 2022): Mr. Rainey was trained on the usage of HPC tools and performing simulations of stratified wake flows.

Project Title: A Low-Cost, Passive Solar Process Heat System
Lead PI: Sungwoo Yang

Students Impacted:

Evan Gildernew (NMX363) is a graduate student pursuing M.S. He has been working on the development of computational modeling for the water harvesting project. He has successfully developed multiple models working. He finds interests on computational research and will pursue Ph.D. program at UTC. The carry over CEACSE grant will support his study.

Syed Tareq is a PhD student who previously worked with Dr. Sou. He decided to stay at UTC working with the PI to complete his PhD study. The part of CEACSE grant will be used to support his PhD study as well.

Project Title: Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss
Lead PI: Sungwoo Yang

Students Impacted:

A PhD student successfully defended his PhD study

UTC Solar Decathlon student club was created where numerous UTC students gain benefits by hand-on experiences on renewable energy research and building technologies

Project Title: Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites
Lead PI: Morgan Smith

Students Impacted:

Two math PhD students, **Carla Adamson** and **Matthew (Gage) Plott** honed programming skills and gained valuable interdisciplinary research experience. Gage developed the initial program and then for personal reasons stepped away from the PhD program (and will return in January). Gage handed the code to Carla at the beginning of the Summer and Carla implemented the flint artifact placement in the layered media along with absorbing boundary conditions on the sides of the computational domain. The plan for Carla is to extend her work this summer into a PhD dissertation, beginning with a PhD doctoral research course with Professor Cox this Fall.

Two Anthropology undergraduate students, **Tyler Mullins** and **Madison Shaw**, acquired experience in viewing and analyzing SONAR datasets for archaeological signatures: experience typically only available to graduate students at other underwater archaeological programs. Madison is now graduated with plans to attend graduate school for anthropology and Tyler, still in our program, gave his first research presentation on the topic at UTC's Spring Research and Arts Conference in 2023 and remains involved in this research.

Project Title: Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy
Lead PI: Lani Gao

Students Impacted:

Two students were enlisted to actively contribute to the progress of this project. **Ms. Gertrude Osei**, a graduate student, received valuable support through the CEACSE grant, where she served as a Research Assistant. Her master's thesis was intricately intertwined with the scope of this research initiative, forming a pivotal component of its execution. Upon the completion of her master's degree, her involvement in this research played a significant role in her successful acceptance into the PhD program in Biostatistics at Indiana University Purdue University Indianapolis in July 2023, underscoring the positive impact of this research experience on her academic journey. The second student, **Mr. James Pritchard**, an undergraduate, also found great value in this research endeavor. His participation contributed to his successful admission to the master's program at the University of Michigan, signifying the project's role in shaping and bolstering students' academic trajectories.

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 from our affiliated faculty's efforts, and direct funding efforts of the CEACSE director and partners.

FY2023 has been another year of growth and enhancement for CEACSE. The leadership team comprises Drs. Joanne Romagni (Vice Chancellor for Research) and Tony Skjellum (former SimCenter Director). Strong collaborative interactions with UTC faculty and administrators underpin this program.

The FY2023 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).

Some notable outcomes in FY2023 include these highlights:

- PI Yang's Ph.D. student successfully defended his dissertation
- PI Gao's graduate student assistant was accepted into a Ph.D. program at Purdue University
- PI Affare participated in a National Science Foundation (NSF) Panel
- PI Alda-Pons' research resulted in the completion of a master's thesis in the department of Biology, Geology, and Environmental Science and established a new researching line at UTC about metabarcoding and the gut microbiome
- PI Alda-Pons' research was published in *Biochemistry and Biophysics Report* and *Biomolecules* and was presented at Vanderbilt's Undergraduate Research Fair, the Association of Southeastern Biologists Annual Meeting in both 2022 and 2023
- PI Ibrahim's project was presented in the International Conference on Metallurgical Coatings and Thin Films and the 14th Symposium on Biodegradable Metal for Biomedical Applications
- PI Manning-Berg's project was presented at the Southeastern-Northcentral Geological Society Meeting and the National Geographic Society Meeting
- PI Ranjan's project resulted in three software products: MINCLES, UTCFOAM, and OS-Solver
- PI Yang received outside funding from both FLY Competition and OCSD
- PI Smith developed FEniCS code as a part of his project

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 seven primary focus areas:

- Advanced Modeling and Simulation
- Critical Infrastructure Protection
- Cybersecurity and Cyber-physical Systems
- Environmental Sustainability and Climate Systems
- Extreme Environment Technologies
- Health and Biological Systems
- High-Performance Computing: Systems & Algorithms

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 in this past cycle underwent rigorous, double-blind, external review with reviewers chosen outside of UTC from among national and international subject matter experts. 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 FY2023/FY2024 as well, and CEACSE awardees are significant producers of external research proposals to several federal agencies and other funding sources.

While these focus areas span a wide area of science and technology, all meritorious research concepts 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.

Overview of FY2023 Projects

For FY2023, these are the projects that were awarded or completed due to extensions from prior years. Six additional projects were funded that have been extended into FY2023 that were mentioned in last year's report as forthcoming and will reported on in next year's report once completed. Delays due to COVID-19 issues and other factors caused these projects to need more time.

The funded projects key to the CEACSE/SimCenter priority areas active in FY2023: Advanced Modeling and Simulation, Critical Infrastructure Protection, Cybersecurity and Cyber-physical Systems, Environmental Sustainability and Climate Systems, Extreme Environment Technologies, Health and Biological Systems, and High-Performance Computing: Systems & Algorithms. Projects could also align with the Center for Urban Informatics and Progress (UTC) priority areas. Not all thrusts are represented in these awards, but certain projects have elements that cross-cut multiple areas.

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.

Initiation/Opportunity Awards

Project Title: “Food Desert Identification and Elimination System”
Lead PI: Sandra Affare
Co-PI(s): N/A

Summary: The purpose of this computational science and engineering project is to develop a web application to support the identification of local areas greatly impacted by limited access to fresh fruit and vegetables. The project’s outcome will be a food desert identification and elimination system. Application of this developed system will foster the development of technology-savvy youth who can solve a real-world problem of limited access to fruit and vegetables in food deserts using computational modeling and simulation. This project proposed to build a computational/GIS model with a front-end interface that will be used to better identify, characterize, and remediate food deserts. It also presents a unique opportunity to address education equity in STEM and promote a successful middle school to college pathway leading to STEM-related careers. If successfully implemented, the proposed project could make significant impacts on food desert research and applications as well as provide a transformative field-based educational model.

Project Title: Molecular modeling of electric double layer and nanoscale heat transfer in supercapacitors
Lead PI: Murat Barisik
Co-PI(s): N/A

Summary: Recent energy storage and conversion applications requires a thorough knowledge of the behavior at electrode/electrolyte interfaces. One of the most promising future technologies, supercapacitors, store energy by building up ionic layers near the electrode surface known as electric double layer (EDL). However, EDL formation through a nanoscale confined electrolyte is not well understood yet. Especially, there is very limited information about the variation of solution temperature during working conditions, and its influence on electric double layer formation. Both ionic layering and heat transfer behavior of a supercapacitor shows non-continuum behavior as the molecular level mechanisms becomes dominant at nano-levels. For the first time in literature, this research project will describe the nanoscale heat transfer and resultant double layer

capacitance based on molecular-level calculations. The Molecular Dynamics (MD) simulations on high-performance computer clusters will be employed, which naturally accounts for molecular nature of both ionic transport and heat transfer. The thermal conductivity of nano-confined electrolytes and interfacial thermal resistance between electrode and electrolyte will be determined. The effects of electrolyte's temperature on the structures of EDL and double layer capacitance will be characterized. Results will be published in a high-impact journal and extended into two extramural grant proposals.

Project Title: Towards Quantum Enhanced Bio-Sensing
Lead PI: Tian Li
Co-PI(s): N/A

Summary: Understanding biological structures and functions relies on our ability to sense and image biological molecules in their native environment, without applying any exogenous labels or modifying the system of interest. Classical sensing is very efficient down to a certain point, where stability and noise start impairing measurements. Sensing below that point (i.e., the standard quantum limit (SQL)), requires sensitivities that can only be achieved with quantum light. Both two-mode squeezed light and entangled photon pairs are ideal sources for producing super-sensitivity in metrology, as has been demonstrated with recent experiments yielding 50% to 70% improvement beyond the SQL. The quantum properties of light, however, have been largely underutilized in biological spectroscopy and imaging. The proposed research program aims at filling those gaps by advancing theoretical, computational, and experimental tools, which exploit quantum optical methods, nonlinear quantum spectroscopy and quantum correlations, to achieve more sensitive, chemically specific, and better resolved optical imaging of biological systems.

Core Competition

Project Title: Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome
Lead PI: Fernando Alda
Co-PI(s): Yu Liang
*** This project was extended from FY2022, and was closed in 2023.

Summary: Biological invasions are a well-recognized threat to biodiversity, human health, and the global economy. Though preventing invasions is often a top management priority, understanding invasion potential is not yet sufficient to predict the likelihood of invasion or to identify regions at risk. Studies suggest that gut microbial diversity and plasticity play a major role in determining invasion potential. So far, all of the evidence supporting the "gut microbial facilitation hypothesis" comes from work on invertebrates. We propose to determine whether it extends to vertebrate invasions and test the hypothesis through the use of deep learning computational analysis to assess whether there are microbial markers of invasive freshwater fishes. Invasive fish can destabilize valued inland fisheries and threaten local biodiversity, especially in global hotspots like the southeastern US. We will use a combination of high throughput sequencing metabarcoding and statistical graphic models to study—in the wild and experimentally—the gut microbiome of native and invasive fishes to (1) test whether there is a signature of invasiveness; and (2) to develop a model that can predict the origin and invasiveness potential of freshwater fishes, which will provide a basis to extrapolate a general theory on the success of biological invasions.

Project Title: From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes
Lead PI: David Giles
Co-PI(s): Steven Symes, Bradley Harris
*** This project was extended from FY2022 and was closed in 2023.

Summary: Bacterial acquisition and utilization of fatty acids represents a pragmatic strategy for survival in various environments. It is now recognized that, in addition to their value as carbon sources, exogenous fatty acids can be recycled and assimilated into membrane phospholipids. The overall objective of this proposal is to investigate the nature of exogenous fatty acid-mediated membrane remodeling and antibiotic resistance in em>Vibrio cholerae. The rationale for the proposed research is that a better understanding of bacterial assimilation of fatty acids, particularly their impact on antibiotic resistance, could be used to manipulate pathogens in clinical and natural settings, resulting in new and innovative approaches for therapeutic intervention and environmental control. A combination of microbiological and biochemical methods are proposed to inform and complement the in silico approach. Computer simulation of membrane dynamics are integral for achieving experimental validity and applicability in predictive potential. This collaborative project represents an interdisciplinary approach, incorporating Biology, Chemistry and Engineering, to address biophysical, biochemical and physiological bacterial membrane dynamics associated with exogenous fatty acid utilization.

Project Title: Topological design of porous metals for biomedical applications
Lead PI: Hamdy Ibrahim
Co-PI(s): Eleni Panagiotou
*** This project was extended from FY2021, and was closed in 2023.

Summary: This proposed research is focused on the creation of optimal biodegradable metal material for biomedical applications using tools from topology. In particular, we focus on the development of such materials for the use in bone implants. It has been shown that the distribution of porosity in bones and their geometry plays a fundamental role in their ability to bear the load of the body. With this research we test the hypothesis that the overall topology of the porous structure, and not only the average size or distance, can provide more refined information to characterize different structures and to provide optimal structures. We will combine computer simulations and topological data analysis, as well as tools from braid theory and graph theoretical approaches. We will propose optimal structures of controlled topology that will be created in the laboratory with established modern techniques, such as 3D printing, and with new methods, such as entangled metal wires. Our approach is expected to provide a new systematic way of studying biodegradable metal material for bone implant applications. This will lead to applications for external funding to study such material at a bigger scale in order to make impacts on medicine and industry.

Project Title: Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants
Lead PI: Hamdy Ibrahim
Co-PI(s): Mohammad Mahtabi
*** This project was extended from FY2022, and was closed in 2023.

Summary: Magnesium and its alloys have been under extensive research recently due to the high potential of their use for biomedical implant applications. For instance, the use of bone implants made of magnesium that can offer the required stability during the healing period and subsequently degrades is expected to result in a clinical breakthrough by eliminating the problems

associated with the standard-of-care permanent implants such as stress shielding. Understanding the corrosion behavior of magnesium-based implants is crucial to assure the biomechanical performance of these new devices. Numerical simulation can serve as a useful tool to reduce the effort needed to achieve that goal. In this study, we propose to develop a numerical model based on the physical modeling approach that is capable of simulating the corrosion behavior of magnesium implants coated with biocompatible ceramic coatings. The developed model will, for the first time, simulate the effect of a ceramic coating layer on the surface of a magnesium-based implant. In vitro corrosion tests under conditions simulating those for the physiological environment will be performed to calibrate and validate the developed model. This model will serve as a future design tool for studying patient-specific biodegradable implants and support our project long-term goals.

Project Title: Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)
Lead PI: Daniel Loveless
Co-PI(s): Donald Reising
*** This project was extended from FY2022, and was closed in 2023.

Summary: Physical authenticity verification of integrated circuits is an unresolved but critical issue for commercial (IoT) and Department of Defense (DoD) systems. Currently, there exists no acceptable way to guarantee that an electronic part is not counterfeit or has not been tampered with, so the concept of "trust" in a mission-critical part, or one that may contain sensitive personal data, may be problematic. The majority of efforts to combat electronic counterfeiting have been focused on the digital layers. However, as wireless connectivity is becoming increasingly prevalent, there is a new opportunity to significantly enhance security through the RF, analog, and mixed-signal layers. This effort introduces a novel tamper forensic technique with the potential to impact all levels of electronics systems through verifiable trust. We will demonstrate a novel, non-destructive post-fabrication imaging technique coupled with RF measurement for initial identification and maintenance of trust through machine learning for enhanced trustworthiness at scale. The proposed activity pushes the boundaries of forensic analysis of the most advanced microelectronic fabrication technology nodes. Given complete development, this proposal's techniques will be applicable across nanometer-scale technologies, address security vulnerabilities at the physical device level, the RF waveform level, and propagate through the digital system level.

Project Title: Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials
Lead PI: Mohamad Mahtabi
Co-PI(s): Hamdy Ibrahim
*** This project was extended from FY2022, and was closed in 2023.

Summary: With the rapid growth in computing power, multiscale simulations are now becoming a viable approach to calculate the properties of materials and design new materials. In this regard, ab initio simulations using Density Functional Theory (DFT), while ideal, are very limited in the size of the model due to computational costs. Molecular dynamics (MD) simulations present a promising alternative to DFT to computationally study the properties of materials. These methods are powerful because deformation properties of materials such as crack initiation and growth, dislocation behavior, polycrystal effects, effects of second phases, interface interactions, and so on, are naturally captured in these simulations. On the other hand, the accuracy of MD simulations heavily relies on the quality of the interatomic potentials. In this proposal, we propose the

development of interatomic potentials, based on multi-objective optimization of parameters to present the mechanical properties of high temperature actuator materials (i.e. high temperature shape memory alloys, HTSMAs). The proposed research involves developing, calibrating, and validating interatomic potentials for MD simulations of alloys made of Ni, Ti, and Hf.

Project Title: Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record
Lead PI: Ashley Manning-Berg
Co-PI(s): N/A
*** This project was extended from FY2022, and was closed in 2023.

Summary: Most of our knowledge of early life on Earth is found in silicified microbial mats, the oldest of which is found in 3.5 billion-year-old rocks composed of silica. The preserved organisms are identified and classified into taxa according to their morphology. However, silicified microfossils display a range of preserved morphologies, from well-preserved to unrecognizable. This range of morphology is the result of biologic decomposition, which is halted once the silicification process begins. Laboratory experiments suggest that morphologic changes occur rapidly during decomposition; therefore, preserved morphologies provide the timing of silica formation and indicate the amount of time an organism experienced decay prior to fossilization. The research proposed will expand on the research previously funded by the mini-CEACSE grant (FY2020) awarded to the PI. The research proposed here will create a way to predict the range of preserved microbial morphologies given a specific length of time that the microbes were exposed to during decomposition. 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.

Project Title: Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2
Lead PI: Hong Qin
Co-PI(s): Ziwei Ma, Azad Hossain
*** This project was extended from FY2022, and was closed in 2023.

Summary: Monitoring adaptive changes of SARS-CoV-2 is of critical importance to mitigate its transmission. Weather temperature and humidity have shown significant statistical associations with the transmission of SARS-CoV-2. Hence, temperature and humidity are proxies of environmental changes for SARS-CoV-2. Our preliminary analyses showed that the D614G mutant prefers drier weather than the reference strain. Genome-wide association study (GWAS) is a typical method to study association between genotype and phenotypic measures. However, GWAS typically requires random sampling. Currently, isolates of SARS-CoV-2 tend to be sequenced in regions with advanced research capacity, and most sequencing were reported during March 2020. These sampling biases pose challenges to genome-wide studies of SARS-CoV-2. Here, we propose to compare a suite of statistical and computational methods to mitigate the sampling biases of SARS-CoV-2, including model-based bootstrap, jackknifing resampling, skew normal distribution, skewed generalized t-distribution, and Gamma distribution. We will compare the accuracy and sensitivity of these methods based on simulation studies, and then apply to investigate the statistical association of nucleotide changes associated with weather temperature and humidity at the county-level. Our proposal will help us better understand the

seasonality of SARS-CoV-2 and contribute to the national and global effort to address the pandemic.

Project Title: Modeling of Transition to Turbulence in Large Eddy Simulation using the Two Level Simulation Approach
Lead PI: Reetesh Ranjan
Co-PI(s): N/A
*** This project was extended from FY2022, and was closed in 2023.

Summary: Transition to turbulence is observed in several aerodynamic applications such as turbomachinery and flow past aircraft wings. Specifically, in wall-bounded flows, transition affects the skin friction coefficient, the wall heat flux, and the spectral and spatio-temporal characteristics. Therefore, an accurate prediction of the onset of transition and the corresponding flow features is important from the design perspective. The presence of such complexities makes the numerical investigation of transitional flows extremely challenging. While direct numerical simulation (DNS) can be used to examine fundamental features of such flows, large-eddy simulation (LES) tends to be more suitable for the investigation of practical applications. However, models for LES are usually derived for fully developed turbulence, thus requiring improved or alternate strategies. The proposed research will establish a hybrid modeling strategy for LES of transitional flows where the two-level simulation (TLS) model, a multi-scale model, is used for near-wall modeling. TLS model does not employ the notion of eddy viscosity, which allows it to capture small-scale physics such as anisotropy, vorticity dynamics, backscatter, and co-/counter-gradient transport. The hybrid modeling strategy will be first assessed through a series of well establish test cases, and then used for further investigation of controlled transition within the boundary layer.

Project Title: Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy
Lead PI: Reetesh Ranjan
Co-PI(s): N/A

Summary: Numerical investigation of stratified turbulent flows observed in engineering and geophysical flows is challenging due to the added complexity of the effects of stratification on turbulence. The challenges are increased further in the flows where differential diffusion effects are present due to the dependence of density stratification on temperature and salinity through a nonlinear equation of state (EoS). Large-eddy simulation (LES) is a computationally tractable approach for the investigation of such flows at practically relevant conditions. However, the subgrid-scale closures used in LES need to be robust and accurate to account for the effects of stratification on the subgrid processes. The proposed research aims to address some of the challenges associated with the modeling of differential diffusion effects in these flows. First, it will examine the effects of moderate levels of differential diffusion at moderate Reynolds number (Re) through direct numerical simulations, where the role of EoS will also be characterized. Secondly, a generalized hybrid multi-scale model leveraging the accuracy of the two-level simulation model and the efficiency of the LES model will be established for predictive LES capabilities. Finally, the established model will be used to study features of high Re axisymmetric towed wake at realistic flow conditions.

Project Title: A Low-Cost, Passive Solar Process Heat System
Lead PI: Sungwoo Yang
Co-PI(s): N/A

*** This project was extended from FY2021, and was closed in 2023.

Summary: Process heating constitutes nearly 70% of the total process energy consumed in the U.S. manufacturing sector, which is almost entirely extracted from fossil fuels. The demand for heating is particularly important for the food processing and beverage industry, which consumes 340 TBtu produced using natural gas annually for process heating. Solar thermal energy is an ideal natural gas substitute for heat generation in the food processing industry. However, the high-cost and complexity of existing concentrated solar-powered industrial process heat systems have prevented their widespread adoption in food processing plants. We propose a low-cost, passive solar process heat system capable of reaching high temperatures and pressures (up to 200 °C, 15 bar) without the need for expensive solar tracking concentrators. The key technological innovation that enables our flat-plate type solar receivers to reach relatively high temperatures relevant for the food processing industry (100-200 °C) is the optically transparent, thermally insulating monolithic silica aerogel developed in our lab. These novel aerogel layers allow transmission of >96% incident solar energy while minimizing heat losses, resulting in efficiencies as high as 75% even without solar concentration.

Project Title: Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss
Lead PI: Sungwoo Yang
Co-PI(s): N/A

Summary: More than a third of all windows in the United States are single-pane windows, which are the most energy-inefficient component of our building envelopes. The annual losses of single-pane windows due to high heat losses is about $12 billion. We propose a one-year project to demonstrate the feasibility of cheap, strong, transparent, insulating (CS-OTTI) retrofits for single-pane windows. A key innovation in our proposed concept is the ability to leverage our ambiently-dried transparent aerogel. It achieves 90% transmittance higher than the best transmittance in literature. We will investigate various novel functionalized silanes to further enhance its optical performance. Our transparent aerogel costs about $1/liter, which is significantly cheaper than conventional aerogel ($3/liter). The monolithic aerogel exhibits reduced effective heat transfer rates (< 0.03 W/mK) without compromising structural integrity. Experimental data and computational modeling will be used to describe thermal performance of the aerogel retrofits on a single-pane window. These innovations have anticipated winter U-factors of < 0.52 BTU/sf/hr/°F, which is close to the performance of expensive air-filled double glazing at significantly lower cost and easy installation. CS-OTTI aerogels will expedite the deployment of OTTI aerogel in practice, including in solar thermal convertors, solar desalination systems, and solar ovens.

Project Title: Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites
Lead PI: Morgan Smith
Co-PI(s): Boris Belinskiy, Abdollah (Abi) Arabshahi

Summary: Our objective is to test, through numerical modeling and simulations, an experimental method of detecting anthropogenic lithic material (stone tools) remotely with a sub-bottom profiler (SBP) as a means of identifying underwater archaeological sites rapidly and non-invasively. We propose to use this funding to work toward the application of a computer code for modelling and simulating this phenomenon, with the eventual goal being to move toward machine learning and automation of this methodology. This project is necessary because the reliability of this method

in the field is unknown, and laboratory tests are needed to control for environmental variables which cannot be mitigated in the field (water temperature, density, turbidity, etc.). However, our project fulfills CEACSE's primary funding goals, as this project concerns modelling, simulation, and machine learning; will result in high-impact peer-reviewed publications; and, if successful, will seed future long-term funding from external sources.

Project Title: Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy
Lead PI: Lani Gao
Co-PI(s): Nagwan Zahry, Ziwei Ma

Summary: We propose a multiscale geographical weighted regression model integrated with Google Trends data analysis (MGWR-GT) to study COVID Vaccine Hesitancy (CVH). MGWR-GT model accounts for common factors association with CVH, as well as geographical and regional specifics of human behavior toward pandemic. The predicted CVH rate can guide COVID vaccine administration and distribution efforts at the state and local levels with consideration of disparities and vulnerable populations. Moreover, reliable and more accurate results given by the model would help public health decision makers respond to the public health crises more quickly, more efficiently, and more effectively. Furthermore, the proposed method can serve as a framework to predict human behavior toward public health crises by integrating traditional data and next-generation dynamic web search data. Finally, this research work will strengthen the real-time data analytics on health-related web queries in this big data era. Our project aims to achieve the following research goals:

- To examine and analyze the factors that influence vaccine hesitancy locally and globally
- To develop a conceptual framework of integrating seasonality of next-generation real-time dynamic data with traditional data analysis
- To explore the vital role of health communication in handling public health crises

FY2023 Budget

NEW CORE AWARDS FY2023				
Lead PI	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Sungwoo Yang	Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss	Energy & Smart Grid	$90,000	$69,336.00
Morgan Smith	Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites	Health and Biological Systems	$99,926	$90,334
Reetesh Ranjan	Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy	Health and Biological Systems; and Advanced Modeling and Simulation	$95,111	$44,453
Lani Gao	Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy	Health and Biological Systems and Advanced Modeling and Simulation	$90,000	$87,120
Meredith Barbee	Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy	Advanced Modeling and Simulation and Health and Biological Systems	$90,000	$37,548**

** *Dr. Barbee was out for a semester for maternity leave and her grant has been extended through 06/30/2024*

Schedule 7

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution: University Of Tennessee Chattanooga **Center:** Applied Computational Science & Engineering

	FY 2022-23 Actual			FY 2023-24 Proposed			FY 2024-25 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries									
Faculty	$107,680	$218,623	**$326,303**	$127,862	$259,598	**$387,460**	$123,234	$250,203	**$373,437**
Other Professional	$27,668	$56,174	**$83,842**	$32,854	$66,703	**$99,556**	$31,664	$64,289	**$95,953**
Clerical/ Supporting	$3,282	$6,663	**$9,945**	$3,897	$7,912	**$11,809**	$3,756	$7,626	**$11,382**
Assistantships	$74,088	$150,421	**$224,509**	$87,974	$178,614	**$266,588**	$84,790	$172,149	**$256,939**
Total Salaries (exclude Longevity)	**$212,717**	**$431,881**	**$644,598**	**$252,586**	**$512,827**	**$765,413**	**$243,445**	**$494,266**	**$737,711**
Longevity (Excluded from Salaries)	$4	$8	**$12**	$5	$10	**$15**	$5	$9	**$14**
Fringe Benefits	$32,530	$66,046	**$98,576**	$38,627	$78,425	**$117,052**	$37,229	$75,586	**$112,815**
Total Personnel	**$245,251**	**$497,935**	**$743,186**	**$291,218**	**$591,261**	**$882,479**	**$280,678**	**$569,862**	**$850,540**
Non-Personnel									
Travel	$15,023	$30,502	**$17,839**	$17,839	$36,218	**$54,057**	$17,193	$34,907	**$52,101**
Software	$1,759	$3,571	**$5,330**	$2,088	$4,240	**$6,329**	$2,013	$4,087	**$6,099**
Other Supplies	$30,148	$61,209	**$91,356**	$35,798	$72,681	**$108,479**	$34,502	$70,050	**$104,553**
Equipment	$42,598	$86,487	**$129,086**	$50,582	$102,697	**$153,280**	$48,752	$98,981	**$147,732**
Maintenance	$1,357	$2,756	**$4,113**	$1,612	$3,272	**$4,884**	$1,553	$3,154	**$4,707**
Scholarships	$15,172	$30,804	**$45,976**	$18,016	$36,577	**$54,593**	$17,364	$35,254	**$52,617**
Other (Specify):									
Printing, Duplicating, Binding	$548	$1,113	**$1,661**	$651	$1,321	**$1,972**	$627	$1,274	**$1,901**
Postage, Freight, & Telephone	$3,581	$7,270	**$10,851**	$4,252	$8,633	**$12,885**	$4,098	$8,320	**$12,418**
Rentals	$2,746	$5,576	**$8,323**	$3,261	$6,621	**$9,883**	$3,143	$6,382	**$9,525**
Publications and Reports	$390	$793	**$1,183**	$464	$941	**$1,405**	$447	$907	**$1,354**
Seminar and Conferences	$3,827	$7,770	**$11,597**	$4,544	$9,227	**$13,771**	$4,380	$8,893	**$13,273**
Student Fees	$14,042	$28,510	**$42,552**	$16,674	$33,853	**$50,527**	$16,071	$32,628	**$48,699**
Special Commercial Services	$1,334	$2,708	**$4,042**	$1,584	$3,216	**$4,800**	$1,527	$3,099	**$4,626**
Other Personal Services	$4,395	$8,923	**$13,318**	$5,219	$10,595	**$15,814**	$5,030	$10,212	**$15,242**
Group Arranged Event	$308	$624	**$932**	$365	$742	**$1,107**	$352	$715	**$1,067**
Other Expenditures	$1,045	$2,122	**$3,167**	$1,241	$2,520	**$3,761**	$1,196	$2,428	**$3,624**
Total Non-Personnel	**$138,274**	**$280,737**	**$391,325**	**$164,190**	**$333,355**	**$497,545**	**$158,247**	**$321,290**	**$479,538**
GRAND TOTAL	**$383,525**	**$778,672**	**$1,134,511**	**$455,408**	**$924,616**	**$1,380,024**	**$438,926**	**$891,152**	**$1,330,078**
Revenue									
New State Appropriation		$850,566	**$850,566**		$880,455	**$880,455**		$924,478	**$924,478**
Carryover State Appropriation			**$0**		$71,894	**$71,894**		$0	**$0**
New Matching Funds	$405,600		**$405,600**	$405,600		**$405,600**	$405,600		**$405,600**
Carryover from Previous Matching Funds			**$0**	$22,075		**$22,075**	$0		**$0**
Total Revenue	**$405,600**	**$850,566**	**$1,256,166**	**$427,675**	**$952,349**	**$1,380,024**	**$405,600**	**$924,478**	**$1,330,078**

FY2023 PUBLICATIONS AND PRESENTATIONS (of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings

Affare, S. and Hunt, N. "Food Desert Identification and Elimination System." UTC Spring Research and Arts Conference. (Non-Refereed Conference), April 2023.

M. Barisik, "Thermal Management of Electric Double-layer Capacitors for Energy Storage Applications" UTC Spring Research and Arts Conference - April 12, 2023.

Matthew Boone (a physics sophomore) will present the results obtained from his summer URP project in the 90th Annual Meeting of Southeastern Section of the American Physical Society, which will be held in Eastern Kentucky University from Nov. 9th to Nov. 11th. (**Tian Li**)

William Hanson-Regan. Geographical, ecological, and genetic drivers of gut microbial diversity in native and invasive minnows of the genus *Cyprinella* (Actinopterygii: Leuciscidae). M.S. Thesis. University of Tennessee at Chattanooga, Chattanooga TN, USA. (**Fernando Alda**)

William Hanson-Regan, Francesca Leasi, **Fernando Alda**. Invasive and Native Fish Microbiomes: Identifying and Comparing the Inhabitants of Fish Guts. The UTC Spring Research and Arts Conference. University of Tennessee at Chattanooga, Chattanooga TN, USA. April 12th-13th 2023.

Saksena, S. & **Giles, D.** Phylogenetic Investigation of Gammaproteobacteria Proteins involved in Exogenous Long-Chain Fatty Acid Acquisition and Assimilation. Vanderbilt Undergraduate Research Fair. Vanderbilt University, Nashville, TN. September 8, 2022.

Patel, N. & **Giles, D.** Polyunsaturated fatty acids affect membrane permeability and antimicrobial activity of polymyxin B and colistin on Vibrio cholerae. Association of Southeastern Biologists Annual Meeting. Poster presentation. Little Rock, AR. March 2022.

Chester, O. & **Giles, D.** The effects of polyunsaturated fatty acids in the presence of piscidins on Vibrio cholerae. Association of Southeastern Biologists Annual Meeting. Poster presentation. Little Rock, AR. March 2022.

Giles, D. MAGA! Make Antibiotics Great Again! Association of Southeastern Biologists Annual Meeting. Oral presentation—Lightning Talk. Winston-Salem, NC. March 2023.

Patel, N. & **Giles, D.** Polyunsaturated fatty acids affect membrane permeability and antimicrobial activity of polymyxin B and colistin on Vibrio cholerae. UTC Research Dialogues. Poster presentation. April 2022.

Morley, L., Turgeson, A. & Harris B. Comparing Vibrio cholerae FadL homologs by simulated docking and knot theory topological measurement. UTC iCompBio REU Final presentations. https://youtu.be/JdA8zGtqQbU (**Giles**)

Saksena, S. & **Giles, D.** Phylogenetic Investigation of Gammaproteobateria Proteins involved in Exogenous Long-chain Fatty Acid Acquisition and Assimilation. UTC iCompBio REU Final presentations. https://youtu.be/XoikOiPCHw8

House, B. Quantifying the Uptake of Exogenous PUFAs in Vibrio cholerae. UTC Chemistry and Physics URP Oral Presentation. Summer 2022. (**Giles**)

House B. C., Lin A., **Giles D. K.,** Symes S. J. K (2022) Polyunsaturated fatty acid incorporation into membrane phospholipids of Aeromonas salmonicida. SERMACS, San Juan Puerto Rico, Oct 2022, Poster.

Ibrahim, H., (2022, June), High-strength and corrosion-controlled magnesium-based bone implants, TechConnect World Conference and Expo, Washington DC.

Ibrahim, H. (2022, October). Biodegradable Magnesium-based Bone Fixation; Alloy Design, Post-fabrication Processes, and Biocompatibility. **Invited talk** in the *Materials Science & Technology (MS&T)*. Pittsburgh, PA.

Vipul Patil, Ron Balanay, Eleni Panagiotou & **Hamdy Ibrahim** (2023, April). Biodegradable Metallic Braided Structures for Biomedical Implant Applications. *UTC Research Dialogue*. Chattanooga, Tennessee.

Ibrahim, H., (2022, June), High-strength and corrosion-controlled magnesium-based bone implants, TechConnect World Conference and Expo, Washington DC.

Ibrahim, H., (2022, May), Preclinical in vitro and in vivo assessment of high-strength and corrosion-controlled magnesium-based bone implants, International Conference on Metallurgical Coatings and Thin Films (ICMCTF), San Diego, CA.

Abdalla, M., Sims, A., Haghshenas, M., Gupta, M., & **Ibrahim, H.** (2021, October). Corrosion assessment of rare earth elements and magnesium-based nanocomposites for bio-implant applications. *Materials Science & Technology*. Columbus, Ohio.

Ibrahim, H. (2022, October). Biodegradable Magnesium-based Bone Fixation; Alloy Design, Post-fabrication Processes, and Biocompatibility. **Invited talk** in the *Materials Science & Technology (MS&T)*. Pittsburgh, PA.

Hash, S., Jia, M., Diaz., W., Elsaadany, M., & **Ibrahim, H.** (2022, October). Magnesium-Based Nanocomposites for Bone Fracture Repair. *Materials Science & Technology (MS&T)*. Pittsburgh, PA.

Billings, C., Abdalla, M., Anderson, D., & **Ibrahim H.** (2022, August). Preclinical biocompatibility assessment of high-strength and corrosion-controlled magnesium-based bone implants. In *14th Symposium on Biodegradable Metals for Biomedical Applications*, Alicante, Spain.

Hash S., Diaz, W., & **Ibrahim, H.** (2022, April). Corrosion assessment of biodegradable magnesium-based nanocomposites. *UTC Research Dialogue*. Chattanooga, Tennessee.

Andre Flores & **Ibrahim, H.** (2023, April). Fabrication and characterization of magnesium-based nanocomposites for bone implant applications. *UTC Research Dialogue*. Chattanooga, Tennessee.

INVITED “Hardening-By-Design Techniques for Analog and Mixed-Signal ASICs,” by **T. D. Loveless**, presented at the 18th International School on the Effects of Radiation on Embedded Systems for Space Applications (SERESSA), CERN, Geneva, Switzerland, Dec. 2022.

INVITED “Space Radiation Effects in Microelectronic Systems,” by **T. D. Loveless**, presented at the Tennessee Technological University, Cookeville, TN, Sept. 2021.

INVITED “Hardening Techniques for Analog and Mixed-Signal Circuits,” by **T. D. Loveless**, presented at the 2021 IEEE Nuclear Space and Radiation Effects Short Course, Virtual, July 2021.

“Supervised Learning and Classification of Single-Event Transient Anomalies,” by T. Peyton, B. Dean, J. L. Carpenter, M. Fadul, D. R. Reising, and **T. D. Loveless** (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.

“Functional Redundancy for Mitigation of SEE in Heterogeneous Computing Systems,” by S. Camp, J. Carpenter, T. Skjellum, D. Reising, and **T. D. Loveless** (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.

“Detection of Single Event Transients in Arbitrary Waveforms Using Statistical Window Analysis,” by J. L. Carpenter and **T. D. Loveless** (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.

“Towards AI-Based Mitigation of SEE,” by **T. D. Loveless,** J. Carpenter, B. Dean, S. Lawrence, R. Young, and D. Reising (2021). 2021 Single Event Effects Symposium. La Jolla, CA (Virtual).

Ataollahi, S. and **Mahtabi, M.J.,** 2022. “A Study on Fatigue Crack Growth in Single-Crystal NiTi Using Molecular Dynamics” IMECE22- International Mechanical Engineering Congress & Exposition-Virtual Conference: October 30 – November 3, 2022.

Ataollahi, S., **Mahtabi, M.J.,** 2022, “Atomistic Simulation of the nano crack growth in superelastic nickel-titanium alloys,” ASTM international E08 committee meeting, November 2nd, New Orleans, USA.

Manning-Berg, Ashley R., Lam, Elizabeth Kathleen., 2022. Decomposition pathways of microbial communities and mats. Geological Society of America Abstracts with Programs. Vol. 54, No. 4, 2022 doi: 10.1130/abs/2022NC-374872

Manning-Berg, Ashley R., Lam, Elizabeth Kathleen., 2022. Taphonomic changes and decomposition pathways of microbial consortiums. Geological Society of America Abstracts with Programs. Vol 54, No. 5. doi: 10.1130/abs/2022AM-381907

Manning-Berg, Ashley R., Lam, Elizabeth K., Riedman, Leigh Anne, Gomes, Maya. 2021. Modern microbial mat taphonomy and its implications on microfossil preservation. Geological Society of America Abstracts with Programs. Vol 53, No. 6. doi: 10.1130/abs/2021AM-371005

Lam, Elizabeth, K., and **Manning-Berg, Ashley**, 2022. Qualifying changes to microbial communities during decomposition to interpret mat morphologies observed in the rock record. Research Dialogues UTC.

S. Thompson, and **R. Ranjan**, “On the effects of differential diffusion and equation of state in stably stratified turbulent channel flow”, APS, DFD, 2022.

R. Ranjan, S. Kim, & **R. Ranjan,** “Hybrid Two-Level and Large-Eddy Simulation of the Wake of a Towed Sphere in Stably Stratified Fluid”, 34th Symposium on Naval Hydrodynamics, 2022.

S. Thompson, and **R. Ranjan**, “One of the effects of differential diffusion and equation of state in stably stratified turbulent channel flow”, Under Preparation for Journal Submission, 2023.

A. Amiri, E. Durant, and R. Ranjan, “Subgrid modeling using deep neural networks for simulation of smooth and rough turbulent channel flows”, Under Preparation for Journal Submission, 2023.Two-Level Simulation of Transition to Turbulence in Wall-Bounded Flows, APS Division of Fluid Dynamics, 2021. (Presenter: M. Young) (**Ranjan**)

Hybrid Two-Level and Kinetic-Eddy Simulation Model for Numerical Investigation of Wall-Bounded Turbulent Flows, AIAA Aviation Forum and Exposition, 2022. (Presenter: E. Durant) (**Ranjan**)

Large-Eddy Simulation of Transition to Turbulence using the Two-Level Simulation Approach, AIAA Aviation Forum and Exposition, 2021. (Presenter: **R. Ranjan**)

Hybrid Two-Level Large-Eddy Simulation of Transition to Turbulence, Research Dialogues, UTC, 2022 (Presenter: M. Young). (**Ranjan**)

Simulation of Laminar-to-Turbulent Transition using Two Level Simulation Model, CECS Tech Symposium, UTC, 2022 (Presenter: M. Young). (**Ranjan**)

Subgrid modeling using deep neural networks for simulation of smooth and rough turbulent channel flows, AIAA Aviation Forum and Exposition, 2023 (Presenter: **R. Ranjan**).

On the effects of differential diffusion and equation of state in stably stratified turbulent channel flow, APS DFD, 2022 (Presenter: S. Thompson). (**Ranjan**)

A. Amiri, and **R. Ranjan**, “Investigation of Reinforcement Learning in Subgrid-Scale Modeling in Large Eddy Simulation”, Spring Research and Arts Conference, UTC, 2023 (Presenter: A. Amiri).

S. Thompson, and **R. Ranjan**, “Numerical Investigation of Physical and Modal Characteristics of Stably Stratified Turbulent Channel Flow”, Spring Research and Arts Conference, UTC, 2023.

A. Amiri, E. Durant, and **R. Ranjan**, “Subgrid modeling using deep neural networks for simulation of smooth and rough turbulent channel flows”, AIAA-2023-3973.

Symposium co-organizer and co-chair: “Re-Visualizing Submerged Landscapes.” Society for Historical Archaeology, Lisbon, Portugal, 2022. (**M. Smith**)

Co-Author: “The Human-Altered Lithic Detection System (HALD) in Real-World Situations, Acoustically Mapping of Submerged Pre-contact Sites in the Gulf of Mexico.” Society for Historical Archaeology, Lisbon, Portugal, 2022. (**M. Smith**)

“Simulation of Wave Propagation Used for the Detection of Submerged Stone Age Artifacts.” Gage Plott, Christopher Cox, Boris Belinskiy, and **Morgan Smith**. UTC Spring Research and Arts Conference, 2023.

Tyler Mullins. “A Cost-Effective Approach to Mapping Submerged Landscapes.” UTC Spring Research and Arts Conference, 2023. (**M. Smith**)

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

2021 ReSEARCH Dialogues and Technology Symposium (**S. Yang**)

2022 ReSEARCH Dialogues and Technology Symposium (**S. Yang**)

Data: Statistical Deep Learning Pilot Study" was presented by PI **Dr. Lani Gao** at Southern Chapter Mathematics Southeastern AMS Sectional Meeting Oct. 15-16, 2022.

“Forecasting COVID-19 Outcomes Using Deep Learning LSTM Models with Google Trends” was presented at conference Symposium on Data Science and Statistics in May 2023. (**L. Gao**)

“Predictive modeling of COVID outcomes Integrating google trend data” was presented by **Dr. Lan Gao** at MATH Colloquium on Nov. 4th, 2022.

Poster: “Forecasting COVID-19 Outcomes Using Deep Learning LSTM Models Using Google Trends” was presented by James Pritchard and Dr. Lan Gao in April 2023. (**L. Gao**)

Software

We are currently in the process of obtaining an open-source license for our IRES code. The possibility of using tools developed using the code, however, will discussed for potential commercialization opportunities. (**Loveless**)

MINCLES: Incompressible flow solver with DNS and LES capabilities for wide range of turbulent flows (**Ranjan**)

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

OS-Solver: A MATLAB based solver for Orr-Sommerfeld equation. (**Ranjan**)

POD/DMD/ANN tools: In-house tools to perform POD/DMD analysis and pre-processing of ANN-based LES closures. (**Ranjan**)

FEniCS code (**M. Smith**)

Refereed Publications

Saksena S., K. Forbes, N. Rajan and **D. Giles**. 2023. Phylogenetic investigation of Gammaproteobacteria proteins involved in exogenous long-chain fatty acid acquisition and assimilation. *Biochem Biophys Rep* 35: 101504. https://doi.org/10.1016/j.bbrep.2023.101504.

Hofer R.N., A. Lin, B.J. House, C.N. Purvis, B.J. Harris, S.J.K. Symes and **D.K. Giles**. 2023. Exogenous polyunsaturated fatty acids (PUFAs) influence permeability, antimicrobial peptide resistance, biofilm formation, and membrane phospholipid structure in A-layer and non-A-layer strains of *Aeromonas salmonicida. J Fish Dis* 46(1):31-45. doi: 10.1111/jfd.13715. Epub 2022 Sep 11.

Turgeson A., L. Morley, **D. Giles** and B. Harris. 2022. Simulated docking predicts putative channels for the transport of long-chain fatty acids in *Vibrio cholerae*. *Biomolecules* 12(9):1269. doi: 10.3390/biom12091269.

Abdalla, M. & **Ibrahim, H.** 2021. A Physical Approach to Simulate the Corrosion of Ceramic-Coated Magnesium Implants. *Applied Sciences*, 11(15), p.6724.

Abdalla, M., Sims, A., Mehanny, S., Haghshenas, M., Gupta, M., & **Ibrahim, H.** (2022). In Vitro Electrochemical Corrosion Assessment of Magnesium Nanocomposites Reinforced with Samarium (III) Oxide and Silicon Dioxide Nanoparticles. Journal of Composites Science, 6(6), 154.

Jia, M. S., Hash, S., Reynoso, W., Elsaadany, M., & **Ibrahim, H.** (2023). Characterization and Biocompatibility Assessment of Boron Nitride Magnesium Nanocomposites for Orthopedic Applications. Bioengineering, 10(7), 757.

Ibrahim, H., Billings, C., Abdalla, M., Korra, A., & Anderson, D. E. (2023). In Vivo Assessment of High-Strength and Corrosion-Controlled Magnesium-Based Bone Implants. Bioengineering, 10(7), 877.

T. Peyton, B. Dean, J. L. Carpenter, M. Fadul, D. R. Reising, and **T. D. Loveless**, "Supervised Learning and Classification of Single-Event Transient Anomalies," IEEE Trans. Nucl. Sci., Apr. 2023.

B. Dean, T. Peyton, J. L. Carpenter, D. Sam, A. Peterson, J. Kim, S. P. Lawrence, M. Fadul, D. R. Reising, and **T. D. Loveless**, "Machine Learning Approaches for Analysis of Total Ionizing Dose in Microelectronics," IEEE RADECS., Oct. 2022.

J. L. Carpenter, B. Dean, S. P. Lawrence, R. D. Young, D. R. Reising, and **T. D. Loveless**, "Analysis of Single Event Transients in Arbitrary Waveforms Using Statistical Window Analysis," IEEE Trans. Nucl. Sci., vol. 70, no. 4, pp. 478-485, Feb. 2023. doi: 10.1109/TNS.2023.3243496.

Ataollahi, S. and **Mahtabi M.J.,** "Atomistic Simulation of Fatigue Crack Growth in Superelastic NiTi" is under preparation to be submitted to "Computational Materials Science" journal.

Lam, Elizabeth K., and **Manning-Berg, Ashley R.,** Taphonomic changes of microorganisms within microbial communities (in prep). Geobiology (IF = 4.2)

M. Young, "Modeling of laminar-to-turbulent transition using a hybrid multi-scale simulation strategy", MS Thesis, UTC, 2022. (**Ranjan**)

E. Durant, M. Young, and **R. Ranjan**, "Hybrid Two-Level and Kinetic-Eddy Simulation Model for Numerical Investigation of Wall-Bounded Turbulent Flows", AIAA-2022-3328, 2022.

R. Ranjan, "Large-Eddy Simulation of Transition to Turbulence using the Two-Level Simulation Approach", AIAA-2021-2892, 2021.

M. Young and **R. Ranjan**, “Large-Eddy Simulation of Laminar to Turbulent using the Two-Level Simulation Approach”, In Preparation, 2022.

Tentative Title “Mathematical Equations for Measuring the Presence of Absence of Materials on the Seafloor.” Target: Journal of Applied Mathematics. Anticipated submission by December, 2023. (**M. Smith**)

Tentative Title “Resonance and Archaeological Site Detection: Possibilities and Problems.” Target: Journal of Archaeological Science. Anticipated submission by January 2024. (**M. Smith**)

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

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

S. Tareq, M. Colson, E. Gildernew, S. Friedman, and **S. Yang**, Enhancing Mechanical Properties of Low Scattering Transparent Insulating Aerogel through Vacuum Packaging and Visualize Insulant Performance, Construction and building materials, Elsevier (in review)

Black, N.; West A.; **Yang, S.**; et. al. Design a Net Zero House at 100-Year Flood Zone in a Historic District: A Case of Solar Decathlon Design Challenge Entry. Journal of Green Building 1 January 2023; 18 (1): 243–263. https://doi.org/10.3992/jgb.18.1.243

Colson, M.; Alvarez, L.; Soto, S. M.; Joo, S. H.; Li, K.; Lupini, A.; Nawaz, K.; Fomunung, I.; Onyango, M. A.; Danquah, M. K.; Owino, J.; **Yang, S.** A Novel Sustainable Process for Multilayer Graphene Synthesis Using CO2 from Ambient Air. Materials 2022, 15 (17), 5894. https://doi.org/10.3390/ma15175894

Gildernew, E.; **Yang, S.**, Finite Element Modeling of Atmospheric Water Extraction by way of Highly Porous Adsorbents: a roadmap for solver construction with model factor sensitivity screening, Journal of Chemical Information and Modeling, 2022 August. https://doi.org/10.1021/acs.jcim.2c00683

Gildernew, E.; Tareq, S.; **Yang, S.** Three-Dimensional Graphene with Preserved Channeling as a Binder Additive for Zeolite 13X for Enhanced Thermal Conductivity, Vapor Transport, and Vapor Adsorption Loading Kinetics, Catalysts 2022, 12(3), 292; https://doi.org/10.3390/catal12030292

“Optimizing Injunctive Norms to increase COVID-19 Vaccination Intention” was submitted to International Journal of Strategic Communication in June 2023. (**L. Gao**)

“Effective COVID-19 Outcome Modeling Using Google Trends Data: A Vector Auto Regression Approach” to be submitted. (**L. Gao**)

Invention Disclosures

Inquiries have been made regarding the potential for developing therapeutics based on this research; however, there is still a substantial amount of work to achieve commercialization. The PI (**Giles**) leveraged this project into applying for a FLY Pitch Competition for Researchers (UTC), in which he won 2nd place and $10,000 to expand and complement this line of research. Furthermore, the preliminary data obtained in the CEACSE also bolstered the PI’s application for a Harris Commercialization Grant (UTC College of Business) that was awarded in the amount of $6,000.

UTRF Invention 23127 was disclosed. (**Hong Qin**)

In-house research codes: OS-Solver, MINCLES, UTCFOAM (**Ranjan**)

UTRF disclosure (UTRF # 21164-02) submitted. (**S. Yang**)

Patent Applications

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

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

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

EXTERNAL FUNDING

Sandra Affare, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Food Desert Identification and Elimination System

Proposal Submissions

- Barbosa, J., Kaplanoglu, E., **Affare, S.** and Zahry, N. "Community-Driven Approach to Food Desert Elimination with STEM-Education & Agricultural Projects" (Agriculture and Food Research Initiative Competitive Grants Program Education and Workforce Development Program Grant submitted March 2023) **$627,426** – *pending.*

Contracts/Awards Received

While the following program was submitted prior to the reporting period, it is immediately related to the awarded CEACSE Mini Grant work.

- "Agriculture and Nutrition for Girls while Encouraging Leadership & STEM-Enrichment" (ANGELS) (submitted to USDA for Women and Minorities in STEM (WAMS) Program Grant, March 2022) Role: Co-PD (PD: Dr. José M. Barbosa) Awarded: **$99,561**

Sponsored Program Capacity Building Activities

- Participated in a National Science Foundation (NSF) Panel – 2022
- NSF stEm PEER Academy Fellow 2022 - 2023
- NSF grant webinars
- Attended UTC Promotion & Tenure Workshop

Murat Barisik, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Molecular Modeling of Electric Double Layer and Nanoscale Heat Transfer in Supercapacitors

Proposal Submissions

- "LEAPS-MPS: Molecular characterization of thermal effects on capacitance behavior of supercapacitors" M Barisik (PI), NSF-LEAPS-MPS $250,000. - *pending*

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

Attended the NSF workshop.

Tian Li, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Towards Quantum Enhanced Bio-Sensing

Proposal Submissions

- DOE ASCR RENEW (invited) - *not funded*
- DOE FAIR (invited) - *withdrawn*
- NSF QuSeC-TAQS (2 preproposals) - *not invited*
- NSF ExpandQISE (full) - *pending*
- NSF ExLENT (full) - *pending*
- NSF Engines (SEQuNA) (full) - *not funded*

Contracts/Awards Received

The proposal to NSF ExLENT (co-PI) has been recommended by NSF.

Sponsored Program Capacity Building Activities

The PI attended the T.I.G. group's NSF Early Career Investigators Workshop hosted by UTC's ORSP

Fernando Alda, Lead PI

Co-PI(s): Yu Liang
Other Personnel: N/A

Project Title: Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome

Proposal Submissions

- N/A

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

- Organizer of the 2nd Southeastern Computational School in RNAseq and Transcriptome Analysis. SimCenter, University of Tennessee at Chattanooga. August 10th-12th, 2022.

David Giles, Lead PI

Co-PI(s): Steven Symes, Bradley Harris
Other Personnel: N/A

Project Title: From in vitro to in silico: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes

Proposal Submissions

- NIH R15. *In vitro and in silico investigations of changes in bacterial cell membrane dynamics due to polyunsaturated fatty acid (PUFA) modifications. $396,750. Submitted June 2023. - pending*

Contracts/Awards Received

- UTC FLY for Researchers 2nd Place Prize ($10,000)
- UTC Harris Commercialization Grant ($6,000)
- UTC Ruth S. Holmberg Grant for Faculty Excellence ($5,000)
- From Previous CEACSE award: Experimentally Guided Modeling and Simulation for Cholera Dynamics. (PI: J. Wang; Co-PIs: D. Giles, B. Harris) $300,000. 2019-2023

Sponsored Program Capacity Building Activities

- The PI participated in a Summer Grant Writing workshop sponsored by the College of Arts and Sciences during summer 2021.

Hamdy Ibrahim, Lead PI

Co-PI(s): Eleni Panagiotou
Other Personnel: N/A

Project Title: Topological design of porous metals for biomedical applications

Proposal Submissions

- E. Panagiotou (UTC), J-M. Carrillo (ORNL), M. Doxastakis (UTK), J. Gounley (ORNL), H. Ibrahim (UTC) & R. Kumar (ORNL) "Topological Material", submitted to the the University of Tennessee-Oak Ridge Innovation Institute (UT-ORII) Seed Funding program, 2021. Requested amount: $62,486. Status: *Not Funded.*

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Hamdy Ibrahim, Lead PI

Co-PI(s): Mohammad Mahtabi
Other Personnel: N/A

Project Title: Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants

Proposal Submissions

- **Ibrahim, H.** “CAREER: CAREER: Hybrid Surface Coating Toward Corrosion-Controlled Magnesium-Based Implants”, submitted to the National Science Foundation (NSF), 2023. Requested amount: $556,776. Status: Pending.

- **Ibrahim, H.**, Dhar, M. & Anderson, D. “Bioactive magnesium implants with controlled degradation and biocompatibility for orthopaedic applications”, CDMRP-IIRA program, submitted to the Department of Defense (DOD), 2023. Total requested amount: $1,913,757, requested amount at UTC: $797,276. Status: Pending.
- **Ibrahim, H.** “ERI: Fabrication and Corrosion Modeling of Biodegradable Synthetic Heart Valves”, submitted to the National Science Foundation (NSF), 2022. Requested amount: $197,175 Status: Not Funded.
- **Ibrahim, H.** “CAREER: Degradation control of coated magnesium toward patient-specific biomedical implants”, submitted to the National Science Foundation (NSF), 2022. Requested amount: $524,289. Status: Not Funded.
- **Ibrahim, H.**, Dhar, M. & Anderson, D. “Bioactive magnesium implants with controlled degradation and biocompatibility for orthopaedic applications”, CDMRP-IIRA program, submitted to the Department of Defense (DOD), 2022. Total requested amount: $1,913,757, requested amount at UTC: $759,264. Status: Not Funded.
- **Ibrahim, H.** “Dissolving and patient-specific Mg-based implants for broken bones”, submitted to the UTC Fly for Researchers 2022 Pitch Competition, 2022. Requested amount: $20,000. Status: **Awarded**.

Contracts/Awards Received

- “Dissolving and patient-specific Mg-based implants for broken bones”, submitted to the UTC Fly for Researchers 2022 Pitch Competition, 2022. Funded amount: $20,000.

Sponsored Program Capacity Building Activities

- N/A

Daniel Loveless, Lead PI

Co-PI(s): Donald Reising
Other Personnel: N/A

Project Title: Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)

Proposal Submissions

1. Missile Defense Agency (MDA) Phase I STTR Sub-contract to CFD Research Corporation, (12/21 – 8/22), Budget: $45,935 (awarded)
2. Missile Defense Agency (MDA) Phase II STTR Sub-contract to CFD Research Corporation, (8/23 – 7/25), Budget: $650,000 (awarded)
3. Defense Threat Reduction Agency (DTRA) IIRM Consortium Member (9/22-12/23), Budget: $185,000 (awarded)

Contracts/Awards Received

1. Missile Defense Agency (MDA) Phase I STTR Sub-contract to CFD Research Corporation, (12/21 – 8/22), Budget: $45,935 (awarded)

2. Missile Defense Agency (MDA) Phase II STTR Sub-contract to CFD Research Corporation, (8/23 – 7/25), Budget: $650,000 (awarded)
3. Defense Threat Reduction Agency (DTRA) IIRM Consortium Member (9/22-12/23), Budget: $185,000 (awarded)

Sponsored Program Capacity Building Activities

1. Partnership with SCALE microelectronics workforce dev program (~$400k funding)
2. Technical chair of NASA NEPP SEE/MAPLD Workshop, La Jolla, CA, 2022
3. Local Arrangements chair of the IEEE NSREC, Provo, Utah, 2022
4. Participant in (1) TAMU Heavy-Ion Training Workshop, (2) NASA NSRL Training Workshop, (3) MSU FRIB Heavy-Ion Testing for DoD, (4) NASA ETW

Mohamad Mahtabi, Lead PI

Co-PI(s): Hamdy Ibrahim
Other Personnel: Mr. Saeed Ataollahi-Graduate Student (Research Assistant), Mr. Mitchell Bauer- Undergraduate Student (Research Assistant), Mr. Stephan Rodemann- Graduate Student (Research Assistant)

Project Title: Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials

Proposal Submissions

1. Mahtabi, M.J. (PI), "Actuation Fatigue and Crack Growth Behavior of Shape Memory Alloys", a collaborative proposal was submitted in October 2022 to NSF's "Metals and Metallic Nanostructures" program, ~$500,000. - *not funded*
2. Mahtabi, M.J. (co-PI), Yang, S. (PI), 2023, "MRI: Acquisition of an Advanced Scanning Transmission Electron Microscopy for Multidisciplinary Research Activities", NSF - National Science Foundation, $999,908 – *not funded*

Contracts/Awards Received

- N/A

Ashley Manning-Berg, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record

Proposal Submissions

- N/A

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

- N/A

Hong Qin, Lead PI

Co-PI(s): Ziwei Ma, Azad Hossain
Other Personnel: N/A

Project Title: Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2

Proposal Submissions

- NSF, CCF 2200138, “PIPP Phase I: Develop and evaluate computational frameworks to predict and prevent future coronavirus pandemics”. PI Qin, Co-PIs Choy, Zhang, Qingge, Ma. Senior personnel: Hossain, Zahry, Heath, Sistrunk - *awarded*

Contracts/Awards Received

- NSF, CCF 2200138, “PIPP Phase I: Develop and evaluate computational frameworks to predict and prevent future coronavirus pandemics”. PI Qin, Co-PIs Choy, Zhang, Qingge, Ma. Senior personnel: Hossain, Zahry, Heath, Sistrunk

Reetesh Ranjan, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Modeling of Transition to Turbulence in Large Eddy Simulation using the Two Level Simulation Approach

Proposal Submissions

1. Towards Physics-Based Modeling of Transition to Turbulence in Wall-Bounded Flows with Predictive Capabilities, NSF CAREER, 2022 (*not funded*) and 2023 (*pending*).
2. Study of Temperature and Three-Dimensional Effects on the Characteristics of Shock-Wave Turbulent Boundary Layer Interaction Using a Novel Hybrid Multi-Scale Modeling Strategy, DEPSCOR, 2021. - *not invited*

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

1. Attended NSF CAREER proposal writing webinar, 2022.
2. Discussion with ONR Program Manager, 2022.

Reetesh Ranjan, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy

Proposal Submissions

1. Numerical Investigation and Multi-Scale Modeling of Differential Diffusion Effects in Stably Stratified Turbulent Flows, Invited Proposal, CHL-10 ERDC, 2023. - *pending*
2. Numerical Investigation and Multi-Scale Modeling of Differential Diffusion Effects in Stably Stratified Turbulent Flows, Accepted Pre-Proposal, CHL-10 ERDC, 2022. - *pending*

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

- N/A

Sungwoo Yang, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: A Low-Cost, Passive Solar Process Heat System

Proposal Submissions

Please list all sponsored program proposals submitted during the reporting period related to this or previous CEACSE awards.

Not funded:

Proposal name	PI or co-PI	External?	Amount requested	Cayuse #
NSF-ERI	PI	Yes	199980	21-4830
ENV-SMART	Co-PI	Yes	443405	21-4466
NSF_MRI	Co-PI	Yes	392000	21-2750
TVA	PI	Yes	150000	21-1225
Ruth S. Holmberg	PI	No	5000	

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

- N/A

Sungwoo Yang, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss

Proposal Submissions

2023	FLY competition - awarded
2023	EnergyTech UP 2023 – not funded
2022	NSF-MRI-FY2023 – not funded
2022	NSF-ERI-FY2023 – not funded
2022	NSF REU-iGREEN – not funded
2022	Search – not funded
2022	OCSD - awarded
2022	NSF S-STEM – not funded
2022	DOE-SIPS – not funded
2022	EREF – not funded
2022	NSF-MRI-FY2022 – not funded

Contracts/Awards Received

2023	FLY competition ($22k)
2022	OCSD ($100k)

Sponsored Program Capacity Building Activities

- N/A

Morgan Smith, Lead PI

Co-PI(s): Boris Belinskiy, Chris Cox
Other Personnel: Gage Plott, Carla Adamson, Tyler Mullins, Maddie Shaw

Project Title: Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites

Proposal Submissions

- Three external proposals were submitted which directly relate to this proposal.
  - “Cultural and Technological Responses to The Early Holocene in the Great Lakes.” The University of Michigan will lead this award, submitted to the NSF Archaeology program. This proposal, submitted in August 2023, would subaward UTC $16,428, - *pending*.
  - “Reevaluating BOEM's Guidelines for Identifying Submerged Pre-Contact Archaeological Sites in the Gulf of Mexico.” Florida State University will lead this award, submitted to the Bureau of Ocean Energy Management. This proposal, submitted in August 2023, would sub-award UTC $99,996 - *pending*.
  - “Using the Tennessee River Near Chattanooga to Revolutionize Methodology and Education in Submerged Precontact Archaeology.” I submitted this first to the CAREER program at NSF and then to the archaeology program with UTC as lead. This proposal, last submitted in February 2023 for $343,121 - *not funded*.

Contracts/Awards Received

- No awards have been received (yet) as a result of this research.

Sponsored Program Capacity Building Activities

This award has built capacity for future research in three primary arenas:

1) Grant funds were used to secure cutting-edge SONAR equipment, including an Innomar SES Compact Parametric Sub-Bottom profiler and an Edgetech 3200 chirp sub-bottom profiler. To my knowledge, UTC is one of perhaps a handful of academic institutions in the country to possess the Innomar system and is certainly the only Anthropology program with one. Having these instruments in our possession not only makes us attractive additions to larger projects (this is already the case with the Florida State University and University of Michigan contracts), but it will make us more competitive for research grants and enhance the skills of our graduates, making them exceptionally qualified for careers in SONAR survey.
2) Grant funds were also used to develop a code from scratch which can be used to rapidly test pressure waves interactions with stone tools in many environments and with many variables. This is crucial, as common critiques of the method, including the effect of environmental variables like salinity, burial substrate, lithic size and shape, etc., can now be tested.
3) Grant funds were also used to build a small acoustic experimentation set-up at UTC, which can be used to move our modelling efforts one step forward into a controlled laboratory environment. Combined with further modelling experiments, these efforts can lay the foundation for further external funding and publication of this exciting research.

Lani Gao, Lead PI

Co-PI(s): Nagwan Zahry, Ziwei Ma
Other Personnel: Gertrude Osei (graduate student worker), James Pritchard (undergraduate student worker)

Project Title: Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy

Proposal Submissions

- We planned to submit a proposal to NSF in Nov. 2023

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

- N/A

OVERVIEW OF FY2024 PROJECTS

The following awardees and projects, selected for funding in February 2023, are currently supporting CEACSE's strategic goals and future plans for FY2023. All funded projects were subject to double-blind external peer review, 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: Modeling heat generation and temperature variation in supercapacitors
Investigator: Murat Barisik
Thrust: Advanced Modeling & Simulation
Amount: $100,000

Abstract: Recent energy storage and conversion applications requires a thorough knowledge of the behavior at electrode/electrolyte interfaces. One of the most promising future technologies, supercapacitors, store energy by building up ionic layers near the electrode surface known as electric double layer (EDL). However, EDL formation through a nanoscale confined electrolyte is not well understood yet. Especially, there is very limited information about the variation of solution temperature during working conditions, and its influence on electric double layer formation. Both ionic layering and heat transfer behavior of a supercapacitor shows noncontinuum behavior as the molecular level mechanisms becomes dominant at nano-levels. For such a case, this research project will study the heat generation and nanoscale heat transfer through electric double layer at molecular level. The Molecular Dynamics (MD) simulations on high-performance computer clusters will be employed, which naturally accounts for molecular nature of both ionic transport and heat transfer. The thermal conductivity of nano-confined electrolytes and interfacial thermal resistance between electrode and electrolyte will be determined. The effects of electrolyte's temperature on the structures of EDL will be measured. Results will be published in two high-impact journal and extended into one extramural grant proposals.

Title: Dynamics Analysis of Online Social Network Models
Investigators: Lingju Kong
Thrust: Advanced Modeling and Simulation
Amount: $96,940

Abstract: In this project, by developing the data-driven deterministic differential equation compartment models, the PI proposes to study the OSN dynamics from two aspects: (a) User traffic dynamics of a single OSN and (b) Competition and coexistence principle of users among multiple OSNs. The proposed project consists of multiple research objectives. The first objective is the development of the user adoption and abandonment model for a single OSN. The model will contain a generalized nonlinear incidence, which is a function of the number of current OSN users. The second objective is to study the competitive exclusion and coexistence of users among multiple OSNs. Due to the physical meanings of the models, conditions for the competitive exclusion and coexistence when one OSN is initially dominant will be the main research focus. Theoretic and numerical analysis will be conducted to understand the model dynamics. The phenomenon of various bifurcations (supercritical, subcritical, or saddle-node, et.al.), sensitivity analysis, and optimal control of the models will also be studied in detail. Case studies combining the developed models and the real-world data will be carried out. These findings will be further applied to predict the evolution of OSN dynamics and derive actionable policies.

Title: Heisenberg-Limited Quantum Sensing Across Entanglement Distributed Quantum Networks
Investigators: Tian Li, Donald Reising
Thrust: Modeling & Simulation of Quantum Systems
Amount: $100,000

Abstract: In this project, we propose to: (1) experimentally demonstrate a table-top continuous-variable entangled quantum network based on a two-mode squeezed state for sensing the average of multiple phase shifts; (2) develop machine learning techniques to measure and control the excess noise distributed across the network, so that Heisenberg-limited parameter estimation can be achieved. Upon completion, our project will be the first experimental realization of machine learning-aided entangled quantum network sensing.

Title: Machine Vision & AI Application for Damaged Solar Panels Detection
Investigators: Abdul Ofoli, Vahid Disfani
Thrust: Critical Infrastructure Protection, including Energy & Smart Grid
Amount: $97,983

Abstract: This project aims to develop machine vision and artificial intelligence solutions to detect damaged solar panels in huge solar farms to (1) increase the reliability of power cultivated from these solar farms and (2) to reduce the maintenance costs of the farms significantly. Solar panels have come a long way, the technology of these free-energy generators is constantly improving. While solar panels are meant to withstand most climates and are built to last 20 to 30 years, they're still not immune to damage especially since they're made from outwardfacing glass. Solar panels can reach their "end-of-life" (EOL) prematurely due to these physical damages and they will need replacements. But most importantly, not being able to capture the state of damaged PV panels can lead to erroneous solar energy forecasting from solar power plants or installations from actual energy productions. Thus, there is a critical need to develop a visual means of inspections and automatic classification of the physical state of installed solar panels to determine healthy and possibly damaged panels.

Title: Creating a Socially Aware Efficient, Transparent, and Equitable 311 System for Smart Cities
Investigators: Yukun Yuan, Joseph Dumas, Junrong Shi, and Prof. Feng Guo
Thrust: Cybersecurity & Cyber-physical Systems
Amount: $99,297

Abstract: Urban 311 services have already been widely used by residents to report non-emergency service requests, e.g., graffiti removal. Researchers have accumulated extensive knowledge on the bias of submitting service requests resulting from persistent spatial, racial, and economic inequalities in cities. However, for residents with diverse social background, studies on the service quality provided by city departments are lacking. This project develops a data driven approach to promote efficient, transparent, and equitable 311 services for diverse communities in a city, by leveraging multi-source data from public socioeconomic and demographic data, city infrastructure, historical service requests, and self-reported survey findings. There are four tasks of this project: i) modeling residents' behavior profile, ii) analyzing community-level social disparity, iii) predicting response time of addressing issues, and iv) designing socially aware learning-based resource scheduling algorithm. Our project has broader impact on both training students and enhancing service quality for residents in real cities.

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 UTC faculty and external collaborators. In coming years, we will also strengthen CEACSE outreach to pre-college students and their teachers (this outreach has been delayed over the past two-plus years by COVID-19).

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 Memoranda of Understanding and Non-Disclosure Agreements have been executed or are in the works 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.

A key related outcome, leveraging the THEC center's computational resources and reputation, is the strong involvement in Exascale computing R&D through the NNSA/DOE-funded Center for Understandable, Performant Exascale Communication Systems (together with the University of New Mexico and University of Alabama), which provides opportunities to enhance the opportunities for students at UTC in high performance computing. This additional funding source and affiliation has led to internships and career opportunities for UTC students in FY2023.

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 FY2023 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.

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 whom 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.

Since then, Tony has accepted a position as a tenured professor at Tennessee Technological University, where he plans to continue his work on both cyber and HPC and Exascale Storage. The CEACSE grant has since been inherited by Dr. Mina Sartipi and the UTC Research Institution.

Dr. Mina Sartipi

Director of the UTC Research Institute
Founding Director of the Center for Urban Informatics and Progress (CUIP)
Guerry Professor of Computer Science and Engineering
Mina-Sartipi@utc.edu

In addition to her roles at UTC, Dr. Sartipi has a joint appointment with the Oak Ridge National Laboratories (ORNL), where she conducts research at the National Transportation Research Center (NTRC). Dr. Sartipi has conducted research on intelligent transportation, data analys, and data acquisition for more than 20 years and has expertise in Smart City applications. She has participated in securing over $14M funding from federal/state/regional government agencies, foundations, and industries in the past few years. These projects cover a variety of applied research related to smart transportation. She is a member of a technical program committee for several workshops and conferences on topics related to AI and smart city operations. Dr. Sartipi was appointed to the Board of Directors of EPB (Electric Power Board) by the Mayor of Chattanooga, which was approved by the City Council in February 2021. She is also a member of several advisory boards including the Board of Trustees for Thrive Regional Partnership, Board of Directors for Chattanooga Urban Studio, and works closely with the Freight Mobility Coalition consisting of 3 states and 16 counties. Dr. Sartipi was named the 2019 Chattanooga Influencer by the Edge, Chattanooga's business magazine, for her role in Smart City research and collaboration with city, county, and industry partners. She has published over 60 papers related to data science, wireless communications, connected vehicles, and data integration. She has delivered several keynotes and presentations including the US Congressional Caucus on Smart Cities, a live demo of connected vehicle projects at the Smart City Connect, and to the National Transportation Training Directions.

Appendix A
Faculty Biosketches

Biographical Sketch

Sandra C. Affare, Ph.D., PMP®, CPEM®, VMA

Adjunct Assistant Professor
The University of Tennessee at Chattanooga
Engineering Management & Technology Department
Sandra-Affare@utc.edu

Executive Summary

- Project Management professional and higher education engineering instructor with an outstanding record of accomplishments in diverse workforces including the federal government, transportation, and logistics
- Champions corporate procedures and project requirements with ethical engineering and project management standards while maintaining a high standard of personal integrity
- Offering more than 15 years of project management oversight and guidance to cross-functional project teams, planning and executing complex projects across multiple departments within an organization.

Education

2016 – Ph.D. Industrial Engineering, University of Tennessee – Knoxville
Dissertation: *High Reliability Organizational Suggestions to Reduce the Risk of Hospital-Associated Infections*

2001 – MBA (Production & Operations Management), University of Tennessee at Chattanooga

1998 – B.S. (Industrial) Engineering, University of Tennessee at Chattanooga

Teaching Experience

2018 – present ***Adjunct Assistant Professor,*** University of Tennessee at Chattanooga (UTC)

2017 – 2021 ***Assistant Professor of Practice,*** UT -Space Institute (UTSI), Tullahoma, TN
Develop engineering pedagogy executing project-based learning for higher education students in Value Management, Strategic Management in Technical Organizations, New Venture Technologies, and Technical Project Management.

Project Management Professional (PMP)® Exam Prep, UTC Continuing Education, SP 2017
Project Management Professional Exam Boot Camp, UTC Continuing Education, Fall 2017

Engineering Design Instructor, Upward Bound Math Science PRISM Program June 2022

Research Proposals Awarded

- **Lead PI** – "Food Desert Identification and Elimination System" (UTC SimCenter CEACSE Mini Grant, May 2022) Awarded: **$14,991**
- **Co-PD** – "Agriculture and Nutrition for Girls while Encouraging Leadership & STEM-Enrichment" (ANGELS) (submitted to USDA for Women and Minorities in STEM (WAMS) Program Grant, March 2022) Awarded: **$99,561**

Service Activity Participated in a National Science Foundation Panel – 2022

License & Certification

Project Management Professional (PMP), Project Management Institute - License # 232398, Expires 16 June 2024

Certified Professional in Engineering Management (CPEM), American Society for Engineering Management - Certification # R15052020CPEM0001, Valid thru 14 June 2025

Professional/ Invited Presentations

"How a Value Engineering Study Can Strategically Improve Your Projects," 2021, PMI Mid-South Professional Development Days, September 2021, Online

"Strategically Improving the Project Plan with Value Methodology," 2020, PMI Mid-South Professional Development Days, September 2020, Online

"HRO Healthcare Research," High Reliability Organization Workshop, 2016, Manchester, TN

Stem for *Her* (Keynote Speaker), March 2023, Chattanooga, TN

Peer-Reviewed Paper Presented

"Analyzing Healthcare Tools Practitioners Use to Implement HRO Theory," Industrial and Systems Engineering Research Conference, 2015, Nashville, TN

Synergistic Activities

- Girl Scout Leader – Developing entrepreneurship and encouraging teambuilding in a girl-led environment. Recently completed "Think Like An Engineer" badges with Girl Scout Brownies (Grades: 1^{st} – 2^{nd}).
- Broadening the participation of underrepresented girls in STEM through mentoring activities.
- Giving talks/lectures aimed at teaching project management skills to students.
- Participated on the Capstone Panel for more than ten (10) students.

Collaborators & Other Affiliations

Lead author and presenter of conference paper, "Analyzing Healthcare Tools Practitioners Use to Implement HRO Theory" in collaboration with:

- Jaime Cantu, Ph.D. (Texas Tech University)
- Janice N. Tolk, Ph.D., P.E. (University of Tennessee Space Institute)

Dissertation Committee:

- James L. Simonton, Ph.D. (University of Tennessee Space Institute) – Co-Chair;
- James Ostrowski, Ph.D. (University of Tennessee - Knoxville)
- Janice N. Tolk, Ph.D., P.E. (University of Tennessee Space Institute)
- Joseph R. Stainback, IV, Ph.D. (University of Tennessee – Knoxville)
- Mingzhou Jin, Ph.D. (University of Tennessee - Knoxville)– Chair
- Yilu Liu, Ph.D. (University of Tennessee – Knoxville)

BIOGRAPHICAL SKETCH

NAME**: Murat Barisik**

POSITION TITLE & INSTITUTION: **Assist. Prof. & UTC Mechanical Engineering**

A. PROFESSIONAL PREPARATION -

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE	YEAR
Middle East Technical University	Ankara/Turkey	Mechanical Engineering	BS	2006
Middle East Technical University	Ankara/Turkey	Mechanical Engineering	MS	2008
Old Dominion University	Norfolk/USA	Aerospace Engineering	PhD	2012
Old Dominion University	Norfolk/USA	Institute of Micro/Nanotechnology	Post-doc	2013

B. APPOINTMENTS

From - To	Position Title, Organization and Location
2022-Present	Assistant Professor, University of Tennessee Chattanooga, USA
2018-2022	Associate Professor, Izmir Institute of Technology, Turkey
2014-2018	Assistant Professor, Izmir Institute of Technology, Turkey
2013-2014	Assistant Research Professor, Southern Methodist University, USA

C. PRODUCTS

(Up to five products most closely related to the proposed project)

1. Yenigün O, Barisik M (2022) Active Heat Transfer Enhancement by Interface-Localized Liquid Dielectrophoresis Using Interdigitated Electrodes. Carbon, 189:339-348.
2. Alan O, Barisik M (2021) Size and Roughness Dependent Temperature Effects on Surface Charge of Silica Nanoparticles, Colloids and Surfaces A: Physicochemical and Engineering Aspects, 629:127407.
3. Yenigün O, Barisik M (2021) Local Heat Transfer Control using Liquid Dielectrophoresis at Graphene/Water Interfaces. International Journal of Heat and Mass Transfer, 166:120801.
4. Sen T, Barisik M (2020) Slip Effects on Ionic Current of Viscoelectric Electroviscous Flows through Different Length Nanofluidic Channels, Langmuir, 36(31):9191–9203. *Selected as the cover art*.
5. Yenigün O, Barisik M (2019) Electric Field Controlled Heat Transfer through Silicon and Nano-confined Water. Nanoscale and Microscale Thermophysical Engineering, 23:304-316.

(Up to five other significant products, whether or not related to the proposed project)

1. Yakin FE, Barisik M, Sen T (2020) Pore Size and Porosity Dependent Zeta Potentials of Mesoporous Silica Nanoparticles, Journal of Physical Chemistry C, 124(36),19579-19587.*Selected as the cover art*.
2. Ozcelik GH, Satiroglu E, Barisik M (2020) Size Dependent Influence of the Contact Line Pinning on Wetting of Nano-textured/patterned Silica Surfaces. Nanoscale, 12:21376-21391.
3. Ozcelik GH, Sozen Y, H Sahin, Barisik M (2020) Parametrizing Nonbonded Interactions between Silica and Water from First Principles. Applied Surface Science, 504, 144359.
4. Alan O, Barisik M, Ozcelik GH (2020) Roughness Effects on Surface Charge Properties of Silica Nanoparticles, Journal of Physical Chemistry C, 124 (13), 7274-7286.
5. Yenigün O, Barisik M (2019) Effect of nano-film thickness on thermal resistance at water/silicon interface. International Journal of Heat and Mass Transfer, 134, 634-640.

NSF BIOGRAPHICAL SKETCH

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Appointments and Positions

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Products

Products Most Closely Related to the Proposed Project

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Other Significant Products, Whether or Not Related to the Proposed Project

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Biographical Sketch

Fernando Alda-Pons, Ph.D.
Assistant Professor

Dpt. Biology, Geology and Enviornmental Science
The University of Tennessee at Chattanooga
351A Holt Hall
Dept. 2653, 615 McCallie Ave.
Chattanooga, TN 37403

(423) 425-2105
fernando-alda@utc.edu; fernandoalda.weebly.com

(a) Professional Preparation

University of Navarra	Pamplona, Spain	Biology	B.Sc., 2002
Complutense University of Madrid	Madrid, Spain	Conservation Biology	M.Sc., 2005
Complutense University of Madrid	Madrid, Spain	Biology	Ph.D., 2009

(b) Appointments

The University of Tennessee at Chattanooga	Chattanooga TN	Assistant Professor	2019-
Louisiana State University	Baton Rouge LA	Postdoctoral Fellow	2015-2018
Tulane University	New Orleans LA	Postdoctoral Researcher	2014-2015
Smithsonian Tropical Research Institute	Panama, Rep. Panama	Postdoctoral Researcher	2012-2014
Institute of Research in Game Resources	Ciudad Real, Spain	Research Scientist	2009-2011

(c) Products *[formerly Publications]*
(i) up to five **products** most closely related to the proposed project

Schönhuth S, Gagne RB, **Alda F**, Neely DA, Mayden RL, Blum MJ (2018) Phylogeography of the widespread Creek Chub *Semotilus atromaculatus* (Cypriniformes: Cyprinoidei). *Journal of Fish Biology* 93: 778-791.

Gagne RB, Sprehn CG, **Alda F**, McIntyre PB, Gilliam JF, Blum MJ. 2017. Invasion pathways and genetic structure of a non-native parasite infecting a native stream fish in Hawai`i. *Ecography* 41: 528-539.

Glotzbecker GJ, **Alda F**, Broughton RE, Neely DA, Mayden RL, Blum MJ. 2016. Geographic independence and phylogenetic diversity of red shiner introductions. *Conservation Genetics* 17: 795-809.

Alda F, Reina RG, Doadrio I, Bermingham E. 2013. Phylogeny and biogeography of the *Poecilia sphenops* species complex (Actinopterygii, Poeciliidae) in Central America. *Molecular Phylogenetics and Evolution* 66: 1011-1026.

Alda F, Ruiz-López MJ, García FJ, Gompper ME, Eggert LS, García JT. 2013. Genetic evidence for multiple introduction events of raccoons (*Procyon lotor*) in Spain. *Biological Invasions* 15: 687-698.

(ii) up to five other significant products, whether or not related to the proposed project.

Alda F, Tagliacollo V, Bernt M, Waltz B, Ludt WB, Faircloth BC, Alfaro ME, Albert JS, Chakrabarty P. 2018. Resolving deep nodes in an ancient radiation of Neotropical fishes in the presence of conflicting signals from incomplete lineage sorting. *Systematic Biology* 68: 573-593.

Faircloth BC, **Alda F**, Hoekzema K, Burns MD, Oliveira C, Albert JS, Melo BF, Ochoa LE, Roxo FF, Chakrabarty P, Sidlauskas BL, Alfaro ME (2018) A target enrichment bait set for studying relationships among ostariophysan fishes. *bioRxiv* 432583: doi: https://doi.org/10.1101/432583.

Chakrabarty P, Faircloth BC, **Alda F**, Ludt WB, McMahan CD, Near TJ, Dornburg A, Albert JS, Arroyave J, Stiassny MLJ, Sorenson L, Alfaro ME. 2017. Phylogenomic systematics of Ostariophysan fishes: ultraconserved elements support the surprising non-monophyly of Characiformes. *Systematic Biology* 66: 881-895.

Burress ED, **Alda F**, Duarte A, Loureiro M, Armbruster JW, Chakrabarty P. 2017. Phylogenomics of the pike cichlids (Cichlidae: *Crenicichla*) and the rapid ecological speciation of an incipient species flock. *Journal of Evolutionary Biology* 31: 14-30.

Picq S, **Alda F**, Krahe R, Bermingham E. 2014. Miocene and Pliocene colonization of the Central American Isthmus by the weakly electric fish *Brachyhypopomus occidentalis* (Hypopomidae, Gymnotiformes). *Journal of Biogeography* 41: 1520-1532.

(d) Synergistic Activities

In my research I aim to answer broad questions in evolutionary biology, by simultaneously expanding fish systematics and evolution, and exploring the best methodologies and practices to accurately and efficiently infer species trees. These strategies mainly involve developing computational strategies for big data analyses. I incorporate these questions in my teaching and outreach activities, and try to reach a broad spectrum of educational levels.

For example, I have been a mentor in a science educational program for Panamanian K12 students under risk of exclusion.

As a university professor, I constantly update my courses with current scientific literature to include real life examples into my lectures. Then, I build on those examples to involve interested undergraduate students in my research and encourage them to publish the work they have carried out in my lab.

For a more specialized audience, either upper level undergraduates or graduate students, I have recently co-organized the 1st Southeastern Computational School at The University of Tennessee at Chattanooga, to educate students in the applications of computational sciences for evolutionary biology.

NAME: Yu Liang

POSITION TITLE & INSTITUTION: Professor, University of Tennessee at Chattanooga

A. PROFESSIONAL PREPARATION
(see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
Tsinghua University	Beijing, China	Computer Science	B.S.	1990
Beijing Polytechnic University	Beijing, China	Computer Science	M.S	1995
Chinese Academy of Science	Beijing, China	Computer Science	Ph.D..	1998
University of Ulster	Coleraine, United Kingdom	Applied Mathematics	Ph.D.	2005
University of Minnesota at Twin Cities	Minneapolis, MN, USA	Computational Science	Post.Doc	2005

B. APPOINTMENTS
(see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
2020-present	Professor / Computer Science, University of Tennessee at Chattanooga. Chattanooga, Tennessee, USA
2013-2020	Associate Professor / Computer Science, University of Tennessee at Chattanooga. Chattanooga, Tennessee, USA
2010-2012	Summer Faculty Fellow / Sensors Directorate, the U.S. Air Force Research Laboratory. Dayton, Ohio, USA
2007-2013	Assistant Professor / Computer Science, Central State University. Dayton, Ohio, USA
2006-2007	Visiting Assistant Professor/Computer Science, Embry-Riddle Aeronautical University, Florida, USA
2005-2006	Research Assistant Professor/Computational Science, North Carolina Agricultural and Technology University, Greensboro, North Carolina, USA

C. PRODUCTS

(see PAPPG Chapter II.C.2.f.(i)(c))

Products Most Closely Related to the Proposed Project

• Y. Liang, D. Wu, Z. Guo, C. Davis, D. Ledesma, and R. Slaughter, "Virtual Tai-Chi, System, a Smart Connected Modality for Rehabilitation", Smart Health, December 2018, 232-249, Vol. 9- 10, DOI: 10.1016/j.smhl.2018.07.021.
• 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.
• 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.

Other Significant Products, Whether or Not Related to the Proposed Project

• Y. Liang, J. Weston and M. Szularz, Generalized Least-squares Polynomial Preconditioners for Symmetric Indefinite Linear Equations. Paralle l 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), 9(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.

D. SYNERGISTIC ACTIVITIES

(see PAPPG Chapter II.C.2.f.(i)(d))

• Panel reviewer for multiple NSF programs, including Graduate Research Fellowships Program (GRFP) since 2015, and NSF OAC Career (2018-2020).
• Program Committee Member for multiple Big-data-related conferences, including Big-data Congress 2019 (July 8-13, 2019, Milan, Italy) and 2020 International Conference on Big Data (Big-data 2020, June 22-26, Honolulu, Hawaii, USA)
• Editorial Board Member for multiple research journals focused on Mathematics and Computer Science.
• Reviewer for 5 journals, including the "Journal of Applied Mathematics and Computer Science."
• Consultant on AI education in middle/high schools for the Hamilton County Department of Education in Chattanooga.

DAVID GILES
University of Tennessee at Chattanooga
Department of Biology, Geology and Environmental Science
Phone: 423-425-2781 Email: david-giles@utc.edu

a. Professional Preparation

- Maryville College, Maryville, TN, Biology, B.A., 2001
- East Tennessee State University, Biomedical Sciences, Ph.D, 2008
- Georgia Health Sciences University, Biochemistry and Molecular Biology, Postdoctoral, 2008-2009
- The University of Texas at Austin, Molecular Genetics and Microbiology, Postdoctoral, 2009-2012

b. Appointments

- Associate Professor, Department of Biology, Geology & Environmental Science, Aug. 2018 – present.
- Assistant Professor, Department of Biology, Geology & Environmental Science, Aug. 2012 – 2018

c. Publications (*undergraduates)

i) Five publications most closely related to proposed project:

- * Saksena S, Forbes K, Rajan N, **Giles D**. 2023. Phylogenetic investigation of Gammaproteobacteria proteins involved in exogenous long-chain fatty acid acquisition and assimilation. *Biochem Biophys Rep* 35: 101504. https://doi.org/10.1016/j.bbrep.2023.101504.
- * Turgeson A, Morley L, **Giles D**, Harris, B. 2022. Simulated docking predicts putative channels for the transport of long-chain fatty acids in *Vibrio cholerae*. *Biomolecules* 12(9):1269. doi: 10.3390/biom12091269.
- * Hofer RN, Lin A, House BJ, Purvis CN, Harris BJ, Symes SJK, **Giles DK**. 2023. Exogenous polyunsaturated fatty acids (PUFAs) influence permeability, antimicrobial peptide resistance, biofilm formation, and membrane phospholipid structure in A-layer and non-A-layer strains of *Aeromonas salmonicida. J Fish Dis* 46(1):31-45. doi: 10.1111/jfd.13715.
- * Smith DS, Houck C, Lee A, Simmons TB, Chester ON, Esdaile A, Symes SJK, **Giles DK**. 2021. Polyunsaturated fatty acids cause physiological and behavioral changes in *Vibrio alginolyticus* and *Vibrio fischeri*. *Microbiologyopen* 10:e1237. doi: 10.1002/mbo3.1237.
- Herndon JL, Peters RE, Hofer RN, Simmons TB, Symes SJ, **Giles DK**. 2020. Exogenous polyunsaturated fatty acids (PUFAs) promote changes in growth, phospholipid composition, membrane permeability and virulence phenotypes in Escherichia coli. *BMC Microbiology* 20:305.

ii) Five other significant publications:

- Hobby CR, Herndon JL, Morrow CA, Symes SJ, **Giles DK**. 2019. Exogenous fatty acids alter phospholipid composition, membrane permeability, capacity for biofilm formation and antimicrobial peptide susceptibility in *Klebsiella pneumoniae*. *MicrobiologyOpen*: e00635.
- Spratt HG, Levine D, Bage J, **Giles DK**, Collier, AG. 2019. Topical lotions utilized in outpatient rehabilitation clinics as a potential source of bacterial contamination. *Physiotherapy Theory and Practice*. 35:163-170.
- Baker LY, Hobby CR, Siv AW, Bible WC, Glennon MS, Anderson DM, Symes SJ, **Giles DK**. 2018. *Pseudomonas aeruginosa* responds to exogenous polyunsaturated fatty acids (PUFAs) by modifying phospholipid composition, membrane permeability, and phenotypes associated with virulence. *BMC Microbiology* 18:117.
- Turgeson A, Boeger R, **Giles DK**, Harris B. 2018. Introducing biochemistry and cellular biology to chemical engineering students by cultivating a bacterial pathogen in a bioreactor. *American Society for Engineering Education-Southeastern Section 2018 Conference Proceedings.* (http://www.asee-se.org/proceedings/ASEE2018/papers2018/3.pdf)

d. Synergistic Activities

- **Campus Representative for Goldwater Scholarship.** Each Fall, Dr. Giles seeks qualifying candidates in natural science, engineering and mathematics for the opportunity of applying for the prestigious Goldwater Scholarship. Dr. Giles reviews applications and provides feedback on student essays during 4 month process. Under his leadership (since 2016), UTC has been awarded 2 Goldwater scholars and 1 Honorable Mention (research student of Dr. Giles).
- **Research mentoring for underrepresented minorities.** Eight of fourteen undergraduate co-authors and trainees are female, and Dr. Giles guided three summer research experiences in Summer 2019 with 4 students (2 female, 2 male; 3 African American, 1 Caucasian). One of these students was awarded the Association of Southeastern Biologists Lafayette Frederick Underrepresented Minorities Scholarship in Spring 2020.
- **Executive Committee member of the Association of Southeastern Biologists (ASB).** Dr. Giles has also served as chair or co-chair of the ASB Poster and Presentation Awards Committee from 2017-2020. Since 2020, he has chaired the Program Committee.
- **Community Outreach.** Dr. Giles has been involved in a variety of events that allow his academic interests to be shared with the local community. He has twice participated in a summer camp for children sponsored by TenneSEA, an environmental organization focused on clean water and children education. Dr. Giles has also given lectures on microbiology/infectious disease for a local homeschool group.
- **Undergraduate Research Advisees:** 35 total since 2018; Four have completed M.S.; 19 undergraduate research advisee co-authors. Dr. Giles is also faculty advisor for the Pre-Optometry Club and TriBeta Biological Honors Society.

BIOGRAPHICAL SKETCH

Provide the following information for the Senior/key personnel and other significant contributors.
Follow this format for each person. **DO NOT EXCEED FIVE PAGES.**

NAME: Steven J. K. Symes, Ph.D.

eRA COMMONS USER NAME (credential, e.g., agency login): SSYMES

POSITION TITLE: UC Foundation Professor of Chemistry

EDUCATION/TRAINING *(Begin with baccalaureate or other initial professional education, such as nursing, include postdoctoral training and residency training if applicable. Add/delete rows as necessary.)*

INSTITUTION AND LOCATION	DEGREE *(if applicable)*	Completion Date MM/YYYY	FIELD OF STUDY
Washington University, St. Louis, MO	B.A.	05/1992	Physics
University of Arkansas, Fayetteville, AR	Ph.D.	08/1996	Analytical Chemistry
NASA Johnson Space Center, Houston, TX	Post-doc	12/1998	Experimental petrology

A. Personal Statement

I am an analytical chemist with >25 years of experience measuring elemental abundances, molecular abundances, and/or isotopic abundances in a wide variety of materials. Recent efforts include: (a) Lipid extractions from bacteria followed by UPLC-MS/MS analysis of phospholipid structures; (b) Metabolite extraction from placental tissue and/or blood samples followed by GC-MS and multi-variate statistical analysis; (c) ICP-MS elemental analyses of placental tissue; (d) GC-MS analysis of placental BPA abundances; and (e) thermal ionization mass spectrometry (TIMS) for ultra-high precision isotopic measurements of Rb, Sr, Sm, and Nd in martian meteorites. I have worked extensively in collaborative settings and my research efforts have been funded by NASA, NSF, US Army, DHHS, and multiple University grants. As a result, I am very skilled at developing and working within a timeline to produce publishable results. All reports and financial accounting required by the various funding agencies have been processed in a timely fashion illustrating my ability to properly administer external and internal funding. I am committed to research with students having directed the research projects of 25 UTC students and served on 4 master's and 10 Departmental Honors committees.

a. Hofer R. N., Lin A, House B. C., Purvis C. N., Harris B. J., **Symes S. J. K.**, Giles D. K. (2023) Exogenous polyunsaturated fatty acids (PUFAs) influence permeability, antimicrobial peptide resistance, biofilm formation and membrane phospholipid structure in an A-layer and non-A-layer strain of *Aeromonas salmonicida*. *J. Fish Dis.*, **46**: 31-45. (Selected for **Cover Art**).

b. Smith D., Houck C., Lee A., Simmons T., Chester O., Esdaile A., **Symes S.**, Giles D. (2021) Polyunsaturated fatty acids cause physiological and behavioral changes in *Vibrio alginolyticus* and *Vibrio fischeri*. *MicrobiologyOpen* 10 (5), e1237.

c. Herndon J., Peters R., Hofer R., Simmons T., **Symes S.**, Giles D. (2020) Exogenous polyunsaturated fatty acids (PUFAs) promote changes in growth, phospholipid composition, membrane permeability and virulence phenotypes in *Escherichia coli*. *BMC Microbiology*, 20:305.

d. Hobby C. R., Herndon J. L., Morrow C. A., Peters R. E., **Symes S. J. K.**, Giles D. K. (2019) Exogenous fatty acids alter phospholipid composition, membrane permeability, capacity for biofilm formation, and antimicrobial peptide susceptibility in *Klebsiella pneumoniae. Microbiology Open*. 2018;e635.

Denotes student co-author

B. Positions, Scientific Appointments, and Honors

2017-present	Professor Department of Obstetrics and Gynecology, UT College of Medicine
Fall 2017	Visiting Scientist, University of Salerno, Salerno, Italy
2012-present	UC Foundation Professor, University of Tennessee at Chattanooga
2010-2011	Visiting Scientist, Lawrence Livermore National Lab, Livermore CA
2010	Panelist reviewer NASA-Lunar Advanced Science and Exploration Research Program
2009-2013	Member, NASA CAPTEM (Curation Analysis Planning Team for Extraterrestrial Materials)
2009 and 2010	Panelist reviewer NASA-Mars Fundamental Research Program
2007 and 2010	Member, NASA MEPAG (Mars Exploration Analysis Group)
2006-2012	UC Foundation Associate Professor, University of Tennessee at Chattanooga
2000-2006	Assistant Professor, University of Tennessee at Chattanooga
1999-2000	Visiting Assistant Professor, University of Tennessee at Chattanooga
1996 – 1998	National Research Council Post-doctoral Fellow; NASA-Johnson Space Center

Honors

2022	UTC Exceptional Merit (4x in last 5 years)
2018	Best Poster award – Association of Southeastern Biologists Meeting, Myrtle Beach SC
2013	Elected to UTC Council of Scholars
2010	University of Tennessee Alumni Association Outstanding Teacher Award
2010	UTC Graduation Commencement Speaker

C. Contributions to Science

Total Publications: >40; for complete list see https://scholar.google.com/citations?user=KuqTfXoAAAAJ&hl=en
Total Citations: > 1600 (h-index = 21)

1. Developed and/or implemented mass spectrometry methods for identification of molecular weight, total number of carbons, and total number of double bonds for phospholipids (PL) and fatty acids derived from Bligh-Dyer extracts of bacterial cultures grown under a variety of conditions: with or without exogenous fatty acids; various growth media; temperatures; and salinity. Extensivlely utilize LipidMaps database (www.lipidmaps.org) to confirm structures. As bacterial membranes are dominated by PE, PG (and CL), negative electrospray ionization quadrupole mass spectrometry with high cone voltage allows unambiguous identification of PL compositions since the cone fragments consist of the cleaved, negatively charged sn-1 and sn-2 acyl moieties. Example publications from this work include:

a. Hofer R. N., Lin A, House B. C., Purvis C. N., Harris B. J., **Symes S. J. K.**, Giles D. K. (2023) Exogenous polyunsaturated fatty acids (PUFAs) influence permeability, antimicrobial peptide resistance, biofilm formation and membrane phospholipid structure in an A-layer and non-A-layer strain of *Aeromonas salmonicida*. *J. Fish Dis.*, **46**: 31-45. (Selected for **Cover Art**).

b. Smith D., Houck C., Lee A., Simmons T., Chester O., Esdaile A., **Symes S.**, Giles D. (2021) Polyunsaturated fatty acids cause physiological and behavioral changes in *Vibrio alginolyticus* and *Vibrio fischeri*. *MicrobiologyOpen* 10 (5), e1237.

c. Herndon J., Peters R., Hofer R., Simmons T., **Symes S.**, Giles D. (2020) Exogenous polyunsaturated fatty acids (PUFAs) promote changes in growth, phospholipid composition, membrane permeability and virulence phenotypes in *Escherichia coli*. *BMC Microbiology*, 20:305.

d. Hobby C. R., Herndon J. L., Morrow C. A., Peters R. E., **Symes S. J. K.**, Giles D. K. (2019) Exogenous fatty acids alter phospholipid composition, membrane permeability, capacity for biofilm formation, and antimicrobial peptide susceptibility in *Klebsiella pneumoniae. Microbiology Open*. 2018;e635.

2. Utilize GC-MS to perform untargeted metabolomics investigations of human serum to look for biomarkers that may be related to a variety of pathologies, including various types of cancer and early-trimester screening for fetal developmental anomalies. Of the various -omics, the metabolome is the closest to the actual phenotype as it unambiguously establishes metabolite patterns at the moment of sampling. Cases and controls for a given pathology are analyzed and results are used to train a variety of machine-learning algorithms to classify subjects. The performance metrics of each algorithm are compared to identify the most useful (i.e., highest AUC of the ROC curve) biomarkers. Blinded clinical trials are employed to test real-world applicability of the trained models.

a. Troisi J., Lombardi M., Scala G., Cavallo P., Tayler R. S., **Symes J.K.**, et al. (2023) A screening test proposal for congenital defects based on maternal serum metabolomics profile. *Am J Obstet Gynecol*. **228 (3)**

b. Troisi J., **Symes S.**, Lombardi M., Cavallo P., et al (2023) Placental metabolomics of fetal growth restriction. *Metabolites* **13**, 235

c. Troisi, Mollo, Lombardi, Scala, Richards, **Symes**, et al. (2022) The metabolomic approach for the screening of endometrial cancer: Validation from a large cohort of women scheduled for gynecological surgery. *Biomolecules* **12**, 1229

d. Troisi J., Tafuro M., Lombardi M., Scala G., Richards S., **Symes S.**, et al. (2022) A Metabolomics-Based Screening Proposal for Colorectal Cancer. *Metabolites* 12 (2), 110.

3. Developed methods for simultaneous determination of a broad mixture of pharmaceuticals in surface waters. The objective of this study was to develop an LC–MS/MS method for the determination of a broad spectrum of commonly used pharmaceuticals in surface water. Further, it was important to make the method as accurate, precise, simple, and cost-effective as possible without compromising sensitivity. To this end, SPE sample pre-concentration coupled with a LC–MS/MS method for separation and detection of 13 different pharmaceuticals and 1 primary metabolite was developed. The utility and ability of this method was applied to samples of surface water collected from the Upper Tennessee River Basin located in eastern Tennessee. Application of this method for the detection of pharmaceuticals in Tennessee River surface water determined that caffeine, sulfamethoxazole, and carbamazepine were frequently detected (100% of samples). Trimethoprim was moderately detected (30% of samples); acetaminophen, atorvastatin, and lovastatin were infrequently detected (10% of samples); and ciprofloxacin, diltiazem, fluoxetine, levofloxacin, norfluoxetine, ranitidine, and sertraline were not detected. This study reported the first detection of lovastatin in surface water.

a. Conley J. M., Schorr M. S., Hanson M.L., **Symes S.J.**, and Richards S. M. (2009) Is ambient chitobiase activity a monitoring tool for impacts on secondary production in lotic systems? *Can. J. Fish. Aquat. Sci.* **66**, 1274.

b. Conley J. M., **Symes S. J.**, Schorr M. S., and Richards S. M. (2008) Spatial and temporal analysis of pharmaceutical concentrations in the upper Tennessee River basin. *Chemosphere* **73**, 1178-1187.

c. Conley J. M., **Symes S. J.**, Kindelberger S. A., and Richards S. M. (2008) Rapid liquid chromatography–tandem mass spectrometry method for the determination of a broad mixture of pharmaceuticals in surface water. *J. Chromatogr. A* **1185**, 206 – 215.

4. Developed methods for ICP analysis of metals in human placenta and co-advised a graduate student who developed method for determining expression of 11β-HSD2 enzyme in human placenta. As a result of this work, I am skilled at tissue digestion and ICP analysis. Results suggest a negative correlation between both Pb and Mn concentration in placenta and resulting birth weight. As placental levels of these elements increase, the birth weight tends to decrease. The enzyme work investigated whether 11β-HSD2 mRNA expression in placental tissue is correlated with birth weight and/or individual birth weight centile in placenta samples collected from Erlanger Hospital in Chattanooga, TN. Additional comparisons were made based on maternal age, marital status, pre-pregnancy body mass index (BMI), race and maternal education to determine if these groupings had any influence on infant birth weight, individual birth weight centile or 11β-HSD2 expression. The following papers relate to these projects:

a. Mikelson C. K., Troisi J., LaLonde A., **Symes S.J.K.**, Thurston S.W., DiRe L.M., Adair C.D., Miller R.K., Richards S.M. (2019) Placental concentrations of essential, toxic, and understudied metals and relationships with birth outcomes in Chattanooga, TN. *Environmental Research*, **168**, 118-129.

b. Mickelson C., Kovach M., Troisi J., **Symes S.**, Adair D., Miller R., Salafia C., Johnson K., Lin Z., and Richards S. (2015) Placental 11β-Hydroxysteroid dehydrogenase type 2 expression: Correlations with birth weight and placental metal concentrations. *Placenta*, **36**, 1212 – 1217.

c. Troisi J., Mikelson C., Richards S., **Symes S.**, Adair D., Zullo F., and Guida M. (2014) Placental concentrations of Bisphenol A and Birth weight from births in the Southeastern U.S. *Placenta*, 947 – 952.

5. Contributed to the understanding of the differentiation of the planet Mars. The goal of this study is to constrain the physical mechanisms by which the shergottites obtain their compositional characteristics. This is accomplished by determining the crystallization age and Sr and Nd isotopic systematics of a mafic martian meteorite Northwest Africa 1195 (NWA1195), thus defining its petrogenetic linkage to other martian meteorites. Then, the compositional variations observed in a subset of martian meteorites are modeled using fractional crystallization algorithms. The success or failure of these models can provide insight into whether fractional crystallization of martian magmas is accompanied by assimilation of martian crust. Ultimately this underscores whether the isotopic variation observed in the broader martian meteorite suite reflects compositional variability in their source regions or the assimilation of evolved crustal material in a martian magma chamber. Our results indicate that NWA1195 has a crystallization age of 347 Ma and initial Sr and Nd isotopic compositions that are very similar to Queen Alexandra Range 94201 (QUE), Dhofar 019, Dar al Gani 476 (DaG), and Yamato 980459 (Y98) suggesting that these meteorites are derived from isotopically very similar source regions. Major and trace element models demonstrate that the compositional variations within this subset of martian meteorites are consistent with fractional crystallization, suggesting that these martian meteorites do not evolve by simple assimilation fractional crystallization. I performed all of the digestions, element separations and purification, and ultra-high precision mass spectrometry using multi-collector thermal ionization MS.

a. **Symes S. J. K.**, Borg L. E., Shearer C. K. and Irving A. J. (2008) The age of the martian meteorite Northwest Africa 1195 and the differentiation history of the shergottites. *Geochim. Cosmochim. Acta* **71**, 1696 – 1710.

b. Borg L. E., Brennecka G. A., and **Symes S. J. K.** (2016) Accretion timescale and impact history of Mars deduced from the isotopic systematics of martian meteorites. *Geochim. Cosmochim. Acta* **175**, 150 – 167.

NAME: Bradley J. Harris

POSITION TITLE & INSTITUTION: Assistant Professor, University of Tennessee Chattanooga

A. PROFESSIONAL PREPARATION
(see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
University of Tennessee, Knoxville	Knoxville, TN	Chemical Engineering	B.S.	2008
University of Tennessee, Knoxville	Knoxville, TN	Chemical Engineering	Ph.D.	2014

B. APPOINTMENTS
(see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
2015 - Present	Assistant Professor, University of Tennessee Chattanooga, Chattanooga, TN
2010 - 2014	Graduate Research Assistant, University of Tennessee Knoxville, Knoxville, TN

C. PRODUCTS

(see PAPPG Chapter II.C.2.f.(i)(c))

Products Most Closely Related to the Proposed Project

1. Turgeson, A., Harris, B. Elucidation of the mechanism of long-chain fatty acid recognition in V. cholerae: an in silico study. American Institute of Chemical Engineers Annual Meeting 2020 November 15-20; San Francisco, CA (accepted).
2. Fomunung, I., Harris, B., et al. ASSETS: Building a Model to Support Transfer Students in Engineering. Frontiers in Education 2020, Uppsala, Sweden, October 21-24 2020 (accepted).
3. Turgeson, A., Boeger, R., Giles, D., and Harris, B. Introducing biochemistry and cellular biology to chemical engineering students by cultivating a bacterial pathogen in a bioreactor. American Society for Engineering Education Southeastern Section Conference, Daytona, FL, March 5 2018. http://www.asee-se.org/proceedings/ASEE2018/2018papersbydivision.htm
4. Harris, B., Cheng, X., and Frymier, P. 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. doi: 10.1021/acs.jpcb.5b07812. PMID: 26671167.
5. Harris, B., Cheng, X., and Frymier, P. All-atom molecular dynamics simulation of a photosystem I/detergent complex. Journal of Physical Chemistry B 2014, 118(40), p. 11633-11645. doi: 10.1021/jp507157e. PubMed PMID: 25233289.

Other Significant Products, Whether or Not Related to the Proposed Project

1. Le, R., Harris, B., Iwuchukwu, I.J., Bruce, B., Cheng, X., Qian, S., Heller, W.T., O'Neill, H., and Frymier, P. Analysis of the solution structure of Thermosynechococcus elongatus photosystem I in n-dodecyl-. -D-maltoside de
2. Harris, B., Le, R., and Frymier, P. Characterizing the structure-function relationship that governs electron transport in redox proteins. Abstracts of Papers of the American Chemical Society 2014, 247.
3. Harris, B. and Frymier, P. Harnessing solar energy through enzyme-mediated protein fusions. Abstracts of Papers of the American Chemical Society 2013, 245.
4. Harris, B. and Dalhaimer, P. Particle shape effects in vitro and in vivo. Frontiers in Bioscience 2012, 4: p. 1344-1353. PubMed PMID: 22652876.

D. SYNERGISTIC ACTIVITIES

(see PAPPG Chapter II.C.2.f.(i)(d))

● Undergraduate research mentorship. Dr. Harris has mentored more than 15 undergraduates, including 4 honors theses and 6 small research grant awardees.
● NSF RET Award # 1953645. Dr. Harris is PI on an RET award providing discovery-based research experiences for community college faculty.
● NIH R15 Award # 1R15GM131315-01A1. Dr. Harris is co-Investigator on an NIH R15 award that aims to establish a new mathematical and computational framework cholera modeling framework.
● NSF S-STEM Award # 1741695. Dr. Harris is co-PI on an S-STEM award for transfer students.
● NSF REU Award # 1852042. Dr. Harris is Senior Personnel on an REU award providing hands-on research experiences and computational biology training to college sophomores and juniors in STEM majors.

Effective 01/30/2023 **NSF BIOGRAPHICAL SKETCH** **OMB-3145-0058**

*NAME Hamdy Ibrahim *Required fields

ORCID ID (Optional)

*POSITION TITLE Assis tant Professor

*PRIMARY ORGANIZATION & LOCATION University of Tennessee at Chattanooga

***PROFESSIONAL PREPARATION - (see PAPPG Chapter II.D.2.h.i.a.3)**

PREVIOUS ORGANIZATION(S) & LOCATION(S)	DEGREE (if applicable)	RECEIPT DATE* (MM/YYYY)	FIELD OF STUDY
University of Toledo	Postdoctoral	2017-2018	Biomedical Eng.
University of Toledo	Ph.D.	2017	Mechanical Eng.
Cairo University	M.S.	2012	Mechanical Eng.
Cairo University	B.S.	2008	Mechanical Eng.

Note - For Fellowship applicants only, please include the start date of the Fellowship.

***APPOINTMENTS AND POSITIONS - (see PAPPG Chapter II.D.2.h.i.a.4)**

Start Date - End Date	Appointment or Position Title, Organization, and Location
Aug. 2018–present	Assistant Professor, Mechanical Engineering, University of Tennessee at Chattanooga, TN
Feb. 2018–July 2018	Chief Research Officer, Thermomorph LLC, Toledo, OH

***PRODUCTS - (see PAPPG Chapter II.D.2.h.i.a.5) Products Most Closely Related to the Proposed Project**

• Delavar, H., Mostahsan, A. J., & Ibrahim, H. (2023). Corrosion and corrosion-fatigue behavior of magnesium metal matrix composites for bio-implant applications: A review. Journal of Magnesium and Alloys.

• Jia, M. S., Hash, S., Reynoso, W., Elsaadany, M., & Ibrahim, H. (2023). Characterization and Biocompatibility Assessment of Boron Nitride Magnesium Nanocomposites for Orthopedic Applications. Bioengineering, 10(7), 757.

• Abdalla, M., & Ibrahim, H. (2021). A Physical Approach to Simulate the Corrosion of Ceramic-Coated Magnesium Implants. Applied Sciences, 11(15), 6724.

• Ibrahim, H., Dehghanghadikolaei, A., Advincula, R., Dean, D., Luo, A., & Elahinia, M. (2019). Ceramic coating for delayed degradation of Mg-1.2 Zn-0.5 Ca-0.5 Mn bone fixation and instrumentation. Thin Solid Films, 687, 137456.

• Ibrahim, H., Esfahani, S. N., Poorganji, B., Dean, D., & Elahinia, M. (2017). Resorbable bone fixation alloys, forming, and post-fabrication treatments. Materials Science and Engineering: C, 70, 870-888.

Other Significant Products, Whether or Not Related to the Proposed Project (see PAPPG Chapter II.D.2.h.i.a.5)

• Ibrahim, H. and Elahinia, M. Heat Treatment Process to Produce High Strength and Corrosion Resistance Mg-Ca-Zn Alloy for Patient-Specific Bioresorbable Bone Fixation Hardware. US20190001027A1, December 21, 2015.

• Cooper J.C., Elahinia, M., Gupta, R. & Ibrahim, H. Minimally Invasive Thrombectomy Device. CIP, US20150265299A1, April 2, 2015.

• Abdalla, M., Sims, A., Mehanny, S., Haghshenas, M., Gupta, M., & Ibrahim, H. (2022). In Vitro Electrochemical Corrosion Assessment of Magnesium Nanocomposites Reinforced with Samarium (III) Oxide and Silicon Dioxide Nanoparticles. Journal of Composites Science, 6(6), 154.

• Abdalla, M., Joplin, A., Elahinia, M., & Ibrahim, H. (2020). Corrosion Modeling of Magnesium and Its Alloys for Biomedical Applications. Corrosion and Materials Degradation, 1(2), 219-248.

• Ibrahim, H., Farag, M., Megahed, H., & Mehanny, S. (2014). Characteristics of starch-based biodegradable composites reinforced with date palm and flax fibers. Carbohydrate polymers, 101, 11-19.

***Synergistic Activities - (see PAPPG Chapter II.D.2.h.(i)(a)(6))**

• Mentored 13 undergraduate and 6 graduate students, guided them through diverse research projects that resulted in significant outcomes, including multiple peer-reviewed publications where students were listed as first authors.

• Guest editor for 3 special issues, including “Engineering Biodegradable-Implant Materials, Volume II" in the journal of Bioengineering – MDPI.

• Participated in the NSF I-Corps program twice within teams consisting of students and researchers. One time as the entrepreneurial lead towards the development and commercialization of a clot removal device. Second time as the technical lead towards the development and commercialization of new bone implants.

• Supervised students in research proposal submissions. Two of my students (one is a female undergraduate student) won the 2020 and 2021 SEARCH Award ($1,000) from the Office for Undergraduate Research and Creative Endeavor at the University of Tennessee.

• Peer reviewer for several esteemed journals, including “Acta Biomaterialia”.

***Certification**:

When the individual signs the certification on behalf of themselves, they are certifying that the information is current, accurate, and complete. This includes, but is not limited to, information related to domestic and foreign appointments and positions. Misrepresentations and/or omissions may be subject to prosecution and liability pursuant to, but not limited to, 18 U.S.C. §§287, 1001, 1031 and 31 U.S.C. §§3729-3733 and 3802.

Signature (Please type out full name): Hamdy Ibrahim Date: 07/21/2023

Biographical Sketch for Eleni Panagiotou

(tenure-track) Assistant Professor Department of Mathematics, University of Tennessee at Chattanooga, TN 37403 423-425-4569 eleni-panagiotou@utc.edu

Professional Preparation

National Technical University of Athens (Greece), Applied Mathematics and Physical Sciences, diploma, 2007
National Technical University of Athens (Greece), Applied Mathematics, M.Sc., 2008
National Technical University of Athens (Greece), Mathematics, Ph. D., 2013

Appointments

Assistant Professor (tenure-track), University of Tennessee, Chattanooga, 2018—present
Program Participant (virtual), Kavli Institute for Theoretical Physics, Santa Barbara, June-July 2020
Visiting Lecturer, University of California, Santa Barbara, 2016—2018
Visiting Assistant Professor, University of California, Santa Barbara, 2013—2016
Researcher, National Technical University of Athens, 2013
Program Participant, Isaac Newton Institute for the Mathematical Sciences, Cambridge, UK, 2012
Visiting Researcher, Swiss Federal Institute of Technology ETH Zurich, 2011–2012

Funding (External, since appointed at UTC)

1. "NSF CAREER: Entanglement of active polymers", National Science Foundation, Division of Materials Research and Division of Mathematical Sciences, 2047587 (PI)
2. "RUI: Computational methods for measuring topological entanglement in polymers", National Science Foundation, Division of Mathematical Sciences, Computational Mathematics, 1913180 (PI)
3. "CC* Compute: A cost-effective 2,048 InfiniBand cluster at UTC for campus research and education", National Science Foundation (co-PI)

10 selected publications out of 25 total (19 published, 2 in press, 4 under review)

Smith, P. and Panagiotou, E., 2021 The second Vassiliev measure of random walks in confined space, *J. Phys. A. Math. Theor.* **55** 095601.

Wang, J. and Panagiotou, E. 2021 The protein folding rate and the topology and geometry of the native state, *Scientific Reports*, (in press)

Panagiotou, E. and Kauffman, L. H., 2021, Vassiliev measures of complexity for open and closed curves in 3-space *Proc. R. Soc. A* **477** 20210440

Herschberg, T., Carrillo, J-M., Sumpter, B. G., Panagiotou, E. and Kumar, R., Topological Effects Near Order-Disorder Transitions in Symmetric Diblock Copolymer Melts,2021, *Macromolecules*,54, 74927499

Baldwin, Q. and Panagiotou E., 2021, The local topological free energy of proteins *J. Theor. Biology*, DOI: 10.1016/j.jtbi.2021.110854

Panagiotou E. and Kauffman L. H., 2020, Knot polynomials of open and closed curves *Proc. R. Soc. A* **476** 20200124

Panagiotou E. and Plaxco, K. W., 2020, A topological study of protein folding kinetics, *Topology of Biopolymers, AMS Contemporary Mathematics Series* **746**, 223

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

Panagiotou E., Millett K. C. and Atzberger P., 2019, Topological Methods for Polymeric Materials: Characterizing the Relationship Between Polymer Entanglement and Viscoelasticity, *Polymers* ,**11** (3), 437.

Panagiotou E. 2015, The linking number in systems with periodic boundary conditions, *J. Comp. Phys.* **300** 533-573.

Teaching (at UTC)

Graduate courses: Numerical Linear Algebra, Numerical Methods for Partial Differential Equa-tions, Applied Knot Theory

Undergraduate courses: Calculus with Analytic Geometry II, Elementary Linear Algebra, Complex Analysis, Numerical Analysis

Individual projects and thesis (UTC students):
Undergraduate students: Philip Smith (Math, co-authored 1 paper), Tom Herschberg (Comp. Sci., co-authored 2 papers), Kyle Pifer (Comp. Sci., co-authored 1 paper), Achok Alier (Bio.), Arielle Beard (Bio.), Peter Zeglen (Math).
Graduate students: Kasturi Barkataki (Math), Masumi Sugiyama (Math), Maame Korsah (Math), Evan Gildernew (Chem. Eng.), Mandya Nagaiah, Hemanth Kumar (Math), Jarod Wright (Math)

Selected synergistic Activities (since appointed at UTC)

1. Leader of the Advanced Modeling and Simulation Thrust of the SimCenter
2. Organization of Special Session "Mathematics of Materials" at the Association of Women in Mathematics (AWM) Research Symposium, IMA, University of Minnesota, Minneapolis
3. Organization of AMS meeting: October 15-16, 2022 (Saturday - Sunday) University of Tennessee at Chattanooga (AMS Fall Southeastern Sectional Meeting) Meeting 1181.
4. Organization of virtual AMS meeting: October 10-11, 2020 (Saturday - Sunday) University of Tennessee at Chattanooga (AMS Fall Southeastern Sectional Meeting) Meeting 1161.
5. Organization of Workshop nr 21w5232, Title: Novel Mathematical Methods in Material Science: Applications to Biomaterials, 6/13/21-6/18/21, Banff International Research Station in Banff, Alberta, Canada.
6. Participation at URTOPS program UTC, 2020-2021 Supervision of Achok Alier and Arielle Beard
7. Participation at NSF REU icompbio program at UTC, summer 2020 Supervision of research of Quenisha Baldwin (Tuskegee University) (co-authored 2 papers)
8. Participation at NSF REU icompbio program at UTC, summer 2021 Supervision of research of Jason Wang (U. Penn, co-authored 1 paper) and Jason Middlebrook (East Tennessee State Univ.).
9. Advisor of the Association of Women in Mathematics (AWM) Student Chapter at UTC.
10. Served at the NSF Comp. Math. Panel, March 2020, March 2021, March 2022.

Effective 01/30/2023 **NSF BIOGRAPHICAL SKETCH** **OMB-3145-0058**

*NAME Mohammad Mahtabi *Required fields

ORCID ID (Optional)

*POSITION TITLE Assistant Professor

*PRIMARY ORGANIZATION & LOCATION University of Tennessee Chattanooga, Chattanooga, TN, USA

***PROFESSIONAL PREPARATION - (see PAPPG Chapter II.D.2.h.i.a.3)**

PREVIOUS ORGANIZATION(S) & LOCATION(S)	DEGREE (if applicable)	RECEIPT DATE* (MM/YYYY)	FIELD OF STUDY
University of Tehran, Tehran, Iran	B.SC	09/2005	Engineering/ Civil
Iran Univ. of Sci. & Tech., Tehran, Iran	M.Sc	05/2008	Engineering/ Civil
Mississippi State University, MS, USA	PhD	05/2017	Engineering/ Mechanical
University of Toledo, OH, USA	Postdoc	08/2018	Engineering/ Mechanical

Note - For Fellowship applicants only, please include the start date of the Fellowship.

***APPOINTMENTS AND POSITIONS - (see PAPPG Chapter II.D.2.h.i.a.4)**

Start Date - End Date	Appointment or Position Title, Organization, and Location
08/2018-present	Assistant Professor, ME Department, UT Chattanooga, TN, USA
09/2017-07/2018	Postdoc, MIME Department, The University of Toledo, OH, USA

***PRODUCTS - (see PAPPG Chapter II.D.2.h.i.a.5) Products Most Closely Related to the Proposed Project**

1. Mahtabi, M.J., Shamsaei, N., Mitchell, M.R., 2015. "Fatigue of Nitinol: The state-of-the-art and ongoing challenges". Journal of the Mechanical Behavior of Biomedical Materials 50, 228-254.
2. Ataollahi, S. and Mahtabi, M.J., 2021. "Effects of Precipitate on the Phase Transformation of Single-Crystal NiTi Alloy under Thermal and Mechanical Loads: A Molecular Dynamics Study." Materials Today Communications, p.102859. DOI: 10.1016/j.mtcomm.2021.102859.
3. Mahtabi, M.J., Stone, T.W., Shamsaei, N., 2018. "Load sequence effects and variable amplitude fatigue of superelastic NiTi". International Journal of Mechanical Sciences 148, 307-315.
4. Mahtabi, M.J., Shamsaei, N., 2017. "Fatigue modeling for superelastic NiTi considering cyclic deformation and load ratio effects". Shape Memory and Superelasticity 3, 250-263.
5. Mahtabi, M.J., Shamsaei, N., 2016. "A modified energy-based approach for fatigue life prediction of superelastic NiTi in presence of tensile mean strain and stress". International Journal of Mechanical Sciences 117, 321-333.

Other Significant Products, Whether or Not Related to the Proposed Project (see PAPPG Chapter II.D.2.h.i.a.5)

1. Bagheri, A., Yadollahi, A., Mahtabi, M.J., Paudel, Y., Vance, E., Shamsaei, N. and Horstemeyer, M.F., 2022. Microstructure-Based MultiStage Fatigue Modeling of NiTi Alloy Fabricated via Direct Energy Deposition (DED). Journal of Materials Engineering and Performance, pp.1-15.
2. Bagheri, A., Mahtabi, M.J., Shamsaei, N., 2018. "Fatigue behavior and cyclic deformation of additive manufactured NiTi". Journal of Materials Processing Technology 252, 440-453.
3. Shayanfard, P., Alarcon, E., Barati, M., Mahtabi, M.J., Kadkhodaei, M., Arbab Chirani, S. and Šandera, P., 2021. "Stress raisers and fracture in shape memory alloys: review and ongoing challenges." Critical Reviews in Solid State and Materials Sciences, pp.1-59. DOI: 10.1080/10408436.2021.1896475.
4. Bayati, P., Jahadakbar, A., Barati, M., Nematollahi, M., Saint-Sulpice, L., Haghshenas, M., Chirani, S.A., Mahtabi, M.J. and Elahinia, M., 2020. "Toward low and high cycle fatigue behavior of SLM-fabricated NiTi: considering the effect of build orientation and employing a self-heating approach. " International Journal of Mechanical Sciences, p.105878.
5. Mahtabi, M.J., Shamsaei, N., 2016. "Multiaxial fatigue modeling for Nitinol shape memory alloys under in-phase loading". Journal of the Mechanical Behavior of Biomedical Materials 55, 236-249.

***Synergistic Activities - (see PAPPG Chapter II.D.2.h.(i)(a)(6))**

(1) Dr. Mahtabi served as a member of the organization committee for several "Advanced Manufacturing, Processing, Characterization, and Modeling of Functional Materials" symposiums of Materials Science & Technology .
(2) He is also a member of the ASTM Collaboration Team WK56674 - Revision of E466 Standard Practice for Conducting Force-Controlled Constant Amplitude Axial Fatigue Tests of Metallic Materials.
(3) Dr. Mahtabi served as a guest editor for Bioengineering Journal's special issue entitled "Engineering Bone-Implant Materials" as well as Journal of Manufacturing and Materials Processing's special issue on "Fatigue and Fracture Mechanics in Additive Manufacturing" .
(4) He is a member of the editorial board of the ASTM Journal of Testing and Evaluation and serves as a reviewer for several high impact journals on mechanics of materials.
(5) Dr. Mahtabi has co/advised three PhD students and six Masters students.

***Certification**:

When the individual signs the certification on behalf of themselves, they are certifying that the information is current, accurate, and complete. This includes, but is not limited to, information related to domestic and foreign appointments and positions. Misrepresentations and/or omissions may be subject to prosecution and liability pursuant to, but not limited to, 18 U.S.C. §§287, 1001, 1031 and 31 U.S.C. §§3729-3733 and 3802.

Signature
(Please type out full name): Mohammadjavad Mahtabi Oghani Date: 01/18/2023

IDENTIFYING INFORMATION:

NAME: Loveless, Daniel

ORCID iD: https://orcid.org/0000-0001-9833-871X

POSITION TITLE: Associate Professor

PRIMARY ORGANIZATION AND LOCATION: Indiana University, Bloomington, Indiana, United States

Professional Preparation:

ORGANIZATION AND LOCATION	DEGREE (if applicable)	RECEIPT DATE	FIELD OF STUDY
Vanderbilt University, Nashville, TN	PHD	2009	Electrical Engineering
Vanderbilt University, Nashville, Tennessee, United States	PHD	06/2007	Electrical Engineering
Georgia Institute of Technology, Atlanta, Georgia, United States	BS	07/2004	Electrical Engineering

Appointments and Positions

2023 - present Associate Professor, Indiana University, Bloomington, Indiana, United States

2019 - 2023 Guerry Professor and UC Foundation Associate Professor, University of Tennessee at Chattanooga, Chattanooga, Tennessee, United States

2017 - 2019 UC Foundation Assistant Professor , University of Tennessee at Chattanooga, Chattanooga, Tennessee, United States

2014 - 2017 Assistant Professor, Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, Tennessee, United States

2013 - 2014 Research Assistant Professor, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, Tennessee, United States

2011 - 2013 Adjunct Assistant Professor, Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, Tennessee, United States

2009 - 2013 Senior Research Engineer, Vanderbilt University, Nashville, Tennessee, United States

2009 - 2010 Instructor, Vanderbilt University, Nashville, Tennessee, United States

Products

Products Most Closely Related to the Proposed Project

1. Lawrence SP, Smith SC, Cannon JM, Reising DR, Loveless TD. "Effects of Total Ionizing Dose on SRAM Physical Unclonable Functions. IEEE Transactions on Nuclear Science. 2022 March; 69(3):349-358. DOI: 10.1109/TNS.2022.3146279
2. Cannon JM, Loveless TD, Estrada R, Boggs R, Lawrence SP, Santos G, McCurdy MW, Sternberg AL, Reising DR, Finzell T, Cannon A. Electrical Measurement of Cell-to-Cell Variation of Critical Charge in SRAM and Sensitivity to Single-Event Upsets by Low-Energy Protons. IEEE Transactions on Nuclear Science. 2021 May; 68(5):815-822. DOI:

10.1109/TNS.2021.3061672

3. Fadul M, Reising D, Loveless TD, Ofoli A. Nelder-Mead Simplex Channel Estimation for the RF-DNA Fingerprinting of OFDM Transmitters Under Rayleigh Fading Conditions. IEEE Transactions on Information Forensics and Security. 2021 January; 16:2381-2396. DOI: 10.1109/TIFS.2021.3054524
4. Loveless TD, Reising DR, Cancelleri JC, Massengill LW, McMorrow D. Analysis of Single Event Transients (SET) using Machine Learning (ML) and Ionizing Radiation Effects Spectroscopy (IRES). IEEE Transactions on Nuclear Science. 2021 January.
5. Patel B, Joplin M, Boggs RC, Reising DR, McCurdy MW, Massengill LW, Loveless TD. Ionizing Radiation Effects Spectroscopy for Analysis of Total-Ionizing Dose Degradation in RF Circuits. IEEE Trans. Nucl. Sci.. 2019 January; 66(1):61-68.

Other Significant Products, Whether or Not Related to the Proposed Project

1. Loveless TD, Jagannathan S, Reece T, Chetia J, Bhuva BL, Massengill LW, Wen S, Wong R, Rennie D. Neutron- and Proton-Induced Single Event Upsets for D- and DICE-Flip/Flop Designs at a 40 nm Technology Node. IEEE Trans. Nucl. Sci.. 2011 June; 58(3):1008-1014.
2. Loveless TD, Alles ML, Ball DR, Warren KM, Massengill LW. Parametric Variability Affecting 45 nm SOI SRAM Single Event Upset Cross-Sections. IEEE Trans. Nucl. Sci.. 2010 December; 57(6):3228-3233.
3. Loveless TD, Massengill LW, Holman WT, Bhuva BL, McMorrow D, Warner J. A Generalized Linear Model for Single Event Transient Propagation in Phase-Locked Loops. IEEE Trans. Nucl. Sci.. 2010 October; 57(5):2933-2947.
4. Loveless TD, Massengill LW, Bhuva BL, Holman WT, Reed RA, McMorrow D, Melinger JS, Jenkins P. A Single-Event-Hardened Phase-Locked Loop Fabricated in 130 nm CMOS. IEEE Trans. Nucl. Sci.. 2007 December; 54(6):2012-2020.
5. Loveless TD, Massengill LW, Bhuva BL, Holman WT, Witulski AF, Boulghassoul Y. A Hardened-by-Design Technique for RF Digital Phase-Locked Loops. IEEE Trans. Nucl. Sci.. 2006 December; 53(6):3432-3438.

Synergistic Activities

1. Five best paper awards: e.g., 2018 ASEE Southeastern Section Annual Conference (undergraduate student), 2017 Annual Conference of the National Collegiate Honors Council (NCHC) (undergraduate student), 2012 Annual Government Microcircuit Applications & Critical Technology Conference (graduate student), 2011 International Reliability Physics Symposium (IRPS) (graduate student), 2011 Annual Government Microcircuit Applications & Critical Technology Conference
2. Awards/Honors: e.g., 2021 Guerry Professorship, 2019 IEEE Nuclear Plasma and Sciences Society (NPSS) Radiation Effects Early Achievement Award, 2017 UC Foundation Professorship, 2015 IEEE Senior Member
3. Invited speaker: e.g., 2022 SERESSA (International School on the Effects of Radiation on Embedded Systems for Space Applications), CERN, Geneva, Switzerland, 2021 Nuclear and Space Radiation Effects Short Course, 2021 NASA Electronics Parts and Packaging ETW, Greenbelt, MD, 2017 SERESSA (International School on the Effects of Radiation on Embedded

Systems for Space Applications), Munich, Germany

4. Conference chairpersonships: e.g., 2020 Nuclear and Space Radiation Effects Conference (Finance Chair), 2022 Nuclear and Space Radiation Effects Conference (Local Arrangements Chair), 2022 Single Event Effects Symposium (Technical Chair), 2023 Single Event Effects Symposium (General Chair)
5. Outreach: e.g., Baylor High School (2017-present)

Certification:

When the individual signs the certification on behalf of themselves, they are certifying that the information is current, accurate, and complete. This includes, but is not limited to, information related to domestic and foreign appointments and positions. Misrepresentations and/or omissions may be subject to prosecution and liability pursuant to, but not limited to, 18 U.S.C. §§ 287, 1001, 1031 and 31 U.S.C. §§ 3729-3733 and 3802.

Certified by Loveless, Daniel in SciENcv on 2023-08-28 18:19:49

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

a. Professional Preparation

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

b. Appointments

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

c. Products

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

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

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

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

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

d. Activities

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

NAME: Ashley Manning-Berg

POSITION TITLE & INSTITUTION: Assistant Professor The University of Tennessee at Chattanooga

A. PROFESSIONAL PREPARATION - (see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
The University of West Georgia	Carrollton, GA	Geology	BS	2009
The University of Tennessee - Knoxville	Knoxville, TN	Geology	MS	2014
The University of Tennessee - Knoxville	Knoxville, TN	Geology	PhD	2018

B. APPOINTMENTS - (see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
August 2019-Present	Assistant Professor, The University of Tennessee at Chattanooga, Chattanooga, Tennessee
August 2018-July 2019	Visiting Assistant Professor, Case Western Reserve University, Cleveland, Ohio
August 2012 - July 2018	Graduate Teaching Assistant, The University of Tennessee - Knoxville, Knoxville, Tennessee
June 2017 - September 2017	Graduate Research Intern, The NASA Jet Propulsion Laboratory, Pasadena, California
May 2013 - August 2013	Geology Intern, ExxonMobil, Houston, Texas
June 2009- December 2011	Research Geologist, US Army Corps of Engineers Engineer Research and Development Center, Vicksburg, Mississippi

C. PRODUCTS - (see PAPPG Chapter II.C.2.f.(i)(c)) Products Most Closely Related to the Proposed Project

Manning-Berg, A.R., Goodman, E., and Kah, L.C. (in revision). Calcitized Evaporites in the Mesoproterozoic Atar Group, Mauritania. Precambrian Research

Manning-Berg, A.R., Selly, T., Bartley, J.K. (2021). Decomposition patterns as a tool for understanding taphonomic history in microfossil assemblages. Geobiology, 00, 1– 17. https://doi.org/10.1111/gbi.12475

Manning-Berg, A.R., Wood, R.S., Williford, K.H., and Kah, L.C 2019. Taphonomic assessment of silicified Mesoproterozoic microbial mats (Special Issue of Geosciences)

Manning, Ashley R., and Bartley, Julie K. 2009. Exploring Algal Morphology during Early Decomposition: Testing Hypotheses Regarding the Proterozoic Fossil Record, Geological Society of America Abstracts with Programs, Vol. 41, No. 1, p. 54

Manning, A.R., and Bartley, Julie K., 2009 Exploring Algal Morphology during Early Decomposition: Connections to Ancient Organic Remains. Georgia Academy of Science Vol. 67, No. 1

Other Significant Products, Whether or Not Related to the Proposed Project

Nabhan, S., Kah, L. C., Mishra, B., Pollok, K., Manning-Berg, A. R., & van Zuilen, M. A. 2021. Structural and chemical heterogeneity of Proterozoic organic microfossils of the ca. 1 Ga old Angmaat Formation, Baffin Island, Canada. Geobiology, 19, 557– 584. https://doi.org/10.1111/gbi.12463

Manning-Berg, Ashley R., Dunham, Jeremy I., Kah, Linda, Tuite, Michael, Williford, Kenneth. 2019. Preservation bias in silicified Proterozoic cyanobacterial mats. Geobiology Society Conference

Manning-Berg, A.R., and Kah, L.C. 2017. Proterozoic microbial mats and their constraints on environments of silicification. Geobiology. 2017; 00:1–15. doi: 10.1111/gbi.12238

D. SYNERGISTIC ACTIVITIES - (see PAPPG Chapter II.C.2.f.(i)(d))

Institute of Origins Science Fellow, Case Western Reserve University	2018-Present
Supervised 7 Undergraduate Researchers in Independent Research	2015-Present (at multiple universities)
Technical Session Chair, Goldschmidt Geochemical Conference	2019
McClung Museum Volunteer	2015-2017
Technical Session Chair, GSA National Meeting	2013

ABDOLLAH (ABI) ARABSHAHI
Research Professor | SimCenter and Computational Science and Engineering
University of Tennessee at Chattanooga | Chattanooga, TN 37403
Tel: 423-425-5485, Fax: 423-425-5517, Email: Abi-arabshahi@utc.edu

A. Professional Preparation:

Mississippi State University	Civil Engineering	BS	1982
Mississippi State University	Aerospace Engineering	MS	1985
Mississippi State University	Aerospace Engineering	PhD	1989

B. Appointments:

2005 – Present	Research Professor University of Tennessee at Chattanooga
2002 – 2005	Associate Research Professor University of Tennessee at Chattanooga
1997 – 2002	Senior Research Associate Applied Research Laboratory, The Pennsylvania State University
1995 – 1997	Research Engineer II, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University
1991 - 1995	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

C. Selected Recent Publications

i) Five publications most closely related to proposed project:

- Boutchuen, A., Zimmerman, D., Arabshahi, A., and Palchoudhury, S., “A Novel In Vitro Computational and Experimental Analysis of Nanoparticle Flow using Hydrogel Channels,” submitted to the Journal of Nanomaterials, September 2019.
- Boutchuen, A., Zimmerman, D., Aich, N., Masud, A.M., Arabshahi, A., and Palchoudhury, S., “Increased Plant Growth with Hematite Nanoparticle Fertilizer Drop and Determining Nanoparticle Uptake in Plants Using Multimodal Approach,” the Journal of Nanomaterials, Volume 2019, Article ID 6890572, June 2019.
- Palchoudhury, S., Arabshahi, A., Gharge, U., Albattah, A., George, O., and Foster, Y., “Integrated Experimental and Computational Fluid Dynamics Approach for Nanoparticle Flow Analysis,” the Journal Physics Letters A, Volume 383, Issue 14, May 2019, Pages 1615-1621.
- 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.
- 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.

ii) Five other significant publications:

- 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.
- Gruetzemacher, R., Arabshahi, A."Effects of Inhalation Transience on Particle Transport Through a CT-Based Human Airway Geometry," IMECE2015-52606, to be presented at International Mechanical Engineering Congress and Exhibition, Houston, TX, November 13-19, 2015.
- 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.
- Whitfield, D. L., Taylor, L. K., Beddhu, M., and Arabshahi, A., "Discretized Newton- Relaxation Solution of the Three-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.
- Arabshahi, A., Janus, J. M., "A Multiblock Compressible Navier-Stokes Flow Solver Applied to Complex Launch Vehicles," *AIAA Journal of Spacecraft and Rockets*, Vol. 41, No. 3, pp. 469-472, May-June 2004.

D. Synergistic Activities:

- SimCenter leadership role in unsteady viscous flow engineering applications, scientific computing, and structured 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 one Undergraduate Honor Student and one MS Student (University of Tennessee at Chattanooga)
- Committee member for 7 MS and 3 PhD students (Mississippi State University) and for 6 MS and 4PhD students and mentor for over 72 Undergraduate Student Researchers (University of Tennessee at Chattanooga)
- Tennessee Higher Education Commission (THEC) Center of Excellence in Applied Computational Science & Engineering (CEACSE) Grant: Dr. Arabshahi (Co-PI) is the recipient of a THEC CEACSE award ($100,000) for his interdisciplinary project combining computational and experimental methods to analyze nanoparticle transport, titled “Investigating the flow of nanodrugs through bio-inspired hydrogel channels.”

IDENTIFYING INFORMATION:

NAME: Qin, Hong

POSITION TITLE: Professor

PRIMARY ORGANIZATION AND LOCATION: University of Tennessee at Chattanooga, Chattanooga, Tennessee, United States

Professional Preparation:

ORGANIZATION AND LOCATION	DEGREE (if applicable)	RECEIPT DATE	FIELD OF STUDY
University of Chicago, Chicago, Illinois, United States	PHD	05/2001	Biochemistry and Molecular Biology
Tsinghua University, Beijing, Not Applicable, N/A, China	MS	04/1994	Biophysics
Tsinghua University, Beijing, Not Applicable, N/A, China	BS	06/1991	Biological Science and Technology
Loyola University of Chicago, Chicago, Illinois, United States	MS	05/2002	Computer Science

Appointments and Positions

2016 - present Professor, University of Tennessee at Chattanooga, Chattanooga, Tennessee, United States

2022 - present Professor, Dept of Comp Sci, Dep of Biol,University of Tennessee at Chattanooga, Chattanooga, Tennessee, United States

2016 - 2022 Associate Professor, Dept of Computer Science, Dept of Biology, University of Tennessee at Chattanooga, Chattanooga, Tennessee, United States

2015 - 2016 Associate Professor, Dept of Biology, Spelman College, Atlanta, Georgia, United States

2009 - 2015 Assistant Professor, Dept of Biology, Spelman College, Atlanta, Georgia, United States

2007 - 2009 Assistant Professor, Dept of Agriculture and Biology, Tuskegee University, Tuskegee, Alabama, United States

2004 - 2006 Research Assistant Professor, Dept of Computational Biology and Biostat, University of Rochester, Rochester, New York, United States

Products

Products Most Closely Related to the Proposed Project

1. Ghafari M, Clark J, Guo HB, Yu R, Sun Y, Dang W, Qin H. Complementary performances of convolutional and capsule neural networks on classifying microfluidic images of dividing yeast cells. PLoS One. 2021;16(3):e0246988. PubMed Central PMCID: PMC7968698.
2. Ghafari M, Whitt C, Hatami P, Yang L, Dang W, Qin H. Estimate Yeast Replicative Lifespan from Time-lapse Microfluidic Images with Object Tracking and Lineage Analysis. 2022 14th International Conference on Computer Research and Development (ICCRD). 2022 January 07. Available from: https://ieeexplore.ieee.org/abstract/document/9730498 DOI:

10.1109/ICCRD54409.2022.9730498

3. Güven E, Akçay S, Qin H. The Effect of Gaussian Noise on Maximum Likelihood Fitting of Gompertz and Weibull Mortality Models with Yeast Lifespan Data. Exp Aging Res. 2019 Mar-Apr;45(2):167-179. PubMed PMID: 30849020.
4. Ledesma DA, Powell CA, Shaw J, Qin H. Enabling automated herbarium sheet image post-processing using neural network models for color reference chart detection. Appl Plant Sci. 2020 Mar;8(3):e11331. PubMed Central PMCID: PMC7073326.
5. Qin H. Estimating network changes from lifespan measurements using a parsimonious gene network model of cellular aging. BMC Bioinformatics. 2019 Nov 20;20(1):599. PubMed Central PMCID: PMC6865033.

Other Significant Products, Whether or Not Related to the Proposed Project

1. Erickson OA, Cole RB, Isaacs JM, Alvarez-Clare S, Arnold J, Augustus-Wallace A, Ayoob JC, Berkowitz A, Branchaw J, Burgio KR, Cannon CH, Ceballos RM, Cohen CS, Coller H, Disney J, Doze VA, Eggers MJ, Farina S, Ferguson EL, Gray JJ, Greenberg JT, Hoffmann A, Jensen-Ryan D, Kao RM, Keene AC, Kowalko JE, Lopez SA, Mathis C, Minkara M, Murren CJ, Ondrechen MJ, Ordoñez P, Osano A, Padilla-Crespo E, Palchoudhury S, Qin H, Ramírez-Lugo J, Reithel J, Shaw CA, Smith A, Smith R, Summers AP, Tsien F, Dolan EL. "How Do We Do This at a Distance?!" A Descriptive Study of Remote Undergraduate Research Programs during COVID-19. CBE Life Sci Educ. 2022 Mar;21(1):ar1. PubMed Central PMCID: PMC9250374.
2. Guo HB, Qin H. Association study based on topological constraints of protein-protein interaction networks. Sci Rep. 2020 Jul 1;10(1):10797. PubMed Central PMCID: PMC7329836.
3. Guo HB, Ghafari M, Dang W, Qin H. Protein interaction potential landscapes for yeast replicative aging. Sci Rep. 2021 Mar 30;11(1):7143. PubMed Central PMCID: PMC8010020.
4. Qin H. Teaching computational thinking through bioinformatics to biology students. ACM SIGCSE Bulletin. 2009 March 04; 41(1):188-191. DOI: 10.1145/1508865.1508932
5. Yan D, Qin H, Wu HY, Chen JY. Editorial: AI-Enabled Data Science for COVID-19. Front Big Data. 2021;4:802452. PubMed Central PMCID: PMC8652065.

Synergistic Activities

1. Inter-disciplinary computational REU: Dr. Qin directs a 10-week summer REU that hosts 10 students per year. The REU research projects include mathematical modeling, computational studies, bioinformatics, molecular dynamics simulations, machine learning, and artificial intelligence for big data.
2. CyberCorps, Scholarship for Service. Dr. Qin manages the UTC scholarship program for cybersecurity in collaboration with Tuskegee University.
3. Biological Big Data: Dr. Qin leads a four-institution project on biology big data, which include offer training bootcamps and workshops on biological big data.
4. YouTube Educational Channel. Dr. Qin's YouTube education channel currently has over 1130 subscribers and over 532,559 views. Educational videos include data science, bioinformatics, molecular biology, experimental techniques, microbiology genetics, etc.
5. Qin is a lead PI of five institution collaborative project that develop deep learning methods to predict and prevent future coronavirus pandemics.

Certification:
When the individual signs the certification on behalf of themselves, they are certifying that the information is current, accurate, and complete. This includes, but is not limited to, information related to domestic and foreign appointments and positions. Misrepresentations and/or omissions may be subject to prosecution and liability pursuant to, but not limited to, 18 U.S.C. §§ 287, 1001, 1031 and 31 U.S.C. §§ 3729-3733 and 3802.

Certified by Qin, Hong in SciENcv on 2023-09-07 16:39:56

Biographical Sketch

Ziwei Ma

Department of Mathematics
University of Tennessee at Chattanooga
E-mail: ziwei-ma@utc.edu, Cell: +1-572-288-5853

(a) Professional Preparation

INSTITUTION	LOCATION	MAJOR AREA OF STUDY	DEGREE (if applicable)	YEAR YYYY
Northwest University	Xi'an	Mathematics	BS	2004
Northwest University	Xi'an	Mathematics	MS	2007
New Mexico State University	Las Cruces, NM	Mathematics	MS	2015
New Mexico State University	Las Cruces, NM	Mathematics/Statistics	PHD	2020

(b) Appointments

2020–present: **Assistant Professor**, University of Tennessee at Chattanooga, Chattanooga, TN

2015–2020: **Teaching/Research Assistant**, New Mexico State University,Las Cruces, NM

(c) Products

Most Closely Related to the Proposed Project

1. **Ma, Ziwei**, Ying-Ju Chen, Tonghui Wang, and Jin Liu. Statistical Inference on location parameter under multivariate skew-normal setting. Communication in Statistics - Simulation and Computation. 2020. DOI:10.1080/03610918.2020.1772300
2. **Ma, Ziwei**, Ben Niu, Tuan Phan, Anne Stensjoen, Chibawanye Ene, Timothy Woodiwiss, Tonghui Wang, Philip Maini, Eric Hollan and Tian, Jianjun. Stochastic growth pattern of untreated human glioblastomas predicts the optimal time for surgery, Scientific Reports 10.1 (2020): 1-13. 2020.
3. **Ma, Ziwei**, Wang, Tonghui. The Plausibility Regions for Shape Parameter under Multivariate Skew-Normal (MSN) Settings Based on Inferential Models (IMs). International Journal of Intelligent Technologies and Applied Statistics, vol. 12, no. 1, 31-47, 2019.
4. **Ma, Ziwei**, Chen, Ying-ju, Wang, Tonghui, Peng, Wuzhen. Inferences on location parameters under skew normal settings, In: "Beyond Traditional Probabilistic Methods in Economics" (V. Kreinovich, N. Trung, and N. Thach Eds.). Springer Nature Switzerland, pp.146-162, 2019.
5. **Ma, Ziwei**, Zhu, Xiaonan, Wang, Tonghui, and Autchariyapanitkul, Kittawit. Joint Plausibility Regions for Parameters of Skew Normal Family. In: International Conference of the Thailand Econometrics Society, pp. 233-245. Springer, Cham, 2018.

Other Significant Publications

6. Mu, Lei, Jia, Zhe, **Ma, Ziwei**, Shen, Fuhui, Sun, Yuekuo, and Zang, Yong . A theoretical prediction framework for the construction of a fracture forming limit curve accounting for fracture pattern transition. International Journal of Plasticity (2020): 102706. 2020
7. Tang, Xiaochen, **Ma, Ziwei**, Hu, Qisong, Tang, Wei. A Real-time Arrhythmia Heartbeats Classification Algorithm using Parallel Delta Modulations and Rotated Linear-Kernel Support Vector Machines, In: IEEE Transactions on Biomedical Engineering, vol. 67, no. 4, pp. 978-986, 2020.

8. Wang, Liang, Wang, Tonghui, Yan, Li, **Ma, Ziwei**. Inference on the Exponentiated Uniform Distribution Under Records, International Journal of Intelligent Technologies and Applied Statistics, vol. 12, no. 1, 67-98, 2019.

9. Zhu, Xiaonan, **Ma, Ziwei** , Wang, Tonghui, and Teetranont, Teerawut. Plausibility regions on the skewness parameter of skew normal distributions based on inferential models. In: Robustness in Econometrics, pp. 267-286. Springer, Cham, 2017.

10. Du, Junli, Yuan, Zhifa, **Ma, Ziwei** , Song, Jiuzhou, Xie, Xiaoli, and Chen, Yulin. "KEGG-PATH: Kyoto encyclopedia of genes and genomes-based pathway analysis using a path analysis model." Molecular bioSystems 10, no. 9 (2014): 2441-2447. 2014.

(d) Synergistic Activities

1. **Conference service:**
   (i) Co-Chair contributed Paper session on Stochastic and Random Processes, Joint Mathematics Meetings 2018, San Diego, CA, January 10–13, 2018.

NAME: Azad Hossain

POSITION TITLE & INSTITUTION: Assistant Professor, The University of Tennessee at Chattanooga

A. PROFESSIONAL PREPARATION

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
University of Dhaka	Bangladesh	Geology	B.Sc.	1995
University of Dhaka	Bangladesh	Geology	M.Sc.	1998
University of Mississippi	Oxford, MS	Geological Engineering	M.S.	2004
University of Mississippi	Oxford, MS	Geological Engineering	Ph.D.	2008
University of Mississippi (NCCHE)	Oxford, MS	Postdoctoral Research on the Application of GIS/Remote Sensing in Computational Hydroscience		2008-2011

B. APPOINTMENTS

From - To	Position Title, Organization and Location
2016- Present	Assistant Professor, Department of Biology, Geology and Environmental Science The University of Tennessee at Chattanooga
2015 – 2016	Visiting Assistant Professor, Department of Geology and Geological Engineering The University of Mississippi
2011–2015	Research Scientist, National Center for Computational Hydroscience and Engineering The University of Mississippi
2010 – 2015	Adjunct Assistant Professor, Department of Geology and Geological Engineering The University of Mississippi
2008 – 2011	Post Doct. Res. Associate, National Center for Computational Hydroscience and Engineering The University of Mississippi
2007 – 2008	Geographic Information Systems Technician The University of Mississippi Geoinformatics Center
1999 – 2001	Remote Sensing and GIS Analyst Center for Environmental and Geographic Information Services. Dhaka, Bangladesh.
1998 – 1999	GIS Consultant Center for Environmental and Geographic Information Services, Dhaka, Bangladesh.

C. PRODUCTS

Products Most Closely Related to the Proposed Project

1. Hall, J. and Hossain, A., 2020, Mapping Urban Growth and Evaluating the Associated Risks for Urban Streams in Chattanooga, Tennessee using GIS and Remote Sensing. Sustainability, 12, 1980.
2. Blanton, R., and Hossain, A, 2020, Mapping the Recovery Process of Vegetation Growth in the Copper Basin, Tennessee Using Remote Sensing Technology. GeoHazards, 2020, 1, 31-43.
3. 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.
4. 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.
5. 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.
6. 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.

Other Significant Products, Whether or Not Related to the Proposed Project

• 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.

D. SYNERGISTIC ACTIVITIES

1. Taught both undergraduate and graduate courses on GIS, remote sensing, and spatial analysis. Also taught undergraduate courses on oceanography, physical geology, historical geology, environmental geology, and engineering analysis.
2. Served on several departmental and university committees including hiring; undergraduate curriculum; graduate program; diversity, inclusion, and equity; undergraduate academic standard; and faculty grant.
3. Reviewed different journal articles and served on editorial and review boards of journals.
4. Reviewed internal grants for UTC and external grants for USGS/NIWR.
5. Helped organizing conference and workshops for NCCHE and School of Engineering of Univ. of Mississippi.

Effective 01/30/2023 **NSF BIOGRAPHICAL SKETCH** **OMB-3145-0058**

*NAME Reetesh Ranjan *Required fields

ORCID ID (Optional)

*POSITION TITLE Assistant Professor

*PRIMARY ORGANIZATION & LOCATION University of Tennessee at Chattanooga, TN, USA

***PROFESSIONAL PREPARATION - (see PAPPG Chapter II.D.2.h.i.a.3)**

PREVIOUS ORGANIZATION(S) & LOCATION(S)	DEGREE (if applicable)	RECEIPT DATE* (MM/YYYY)	FIELD OF STUDY
Georgia Institute of Technology, Atlanta, GA, USA	Postdoc	1/2013-6/2015	Aerospace Engineering
University of Illinois, Urbana-Champaign, IL, USA	PhD	12/2012	Theoretical and Applied Mechanics
University of Illinois, Urbana-Champaign, IL, USA	MS	5/2009	Theoretical and Applied Mechanics
Indian Institute of Technology, Kanpur, India	B Tech	5/2004	Mechanical Engineering

Note - For Fellowship applicants only, please include the start date of the Fellowship.

***APPOINTMENTS AND POSITIONS - (see PAPPG Chapter II.D.2.h.i.a.4)**

Start Date - End Date	Appointment or Position Title, Organization, and Location
8/2019 - present	Assistant Professor, University of Tennessee at Chattanooga
7/2019	Senior Research Engineer, School of Aerospace Engineering, Georgia Institute of Technology
7/2015 - 6/2019	Research Engineer II, School of Aerospace Engineering, Georgia Institute of Technology
8/2007-12/2012	Graduate Research Assistant, Mechanical Science & Engineering, University of Illinois
7/2004-7/2007	Lead Application Engineer, Ansys India

***PRODUCTS - (see PAPPG Chapter II.D.2.h.i.a.5) Products Most Closely Related to the Proposed Project**

1. Ranjan, R., & Menon, S. (2013). A multi-scale simulation method for high Reynolds number wall-bounded turbulent flows. Journal of Turbulence, 14(9), 1-38.

2. R. Ranjan, & S. Menon (2018). Vorticity, backscatter and counter-gradient transport predictions using two-level simulation of turbulent flows. Journal of Turbulence, 19(4), 334-364.

3. Ranjan, R., Venkataswamy, M. K., & Menon, S. (2020). Dynamic one-equation-based subgrid model for large-eddy simulation of stratified turbulent flows. Physical Review Fluids, 5(6), 064601.

4. R. Ranjan (2021). Large-Eddy Simulation of Transition to Turbulence using the Two-Level Simulation Approach. AIAA-2021-2892, 2021.

5. E. Durant, M. Young, M., & R. Ranjan (2022). Hybrid Two-Level and Kinetic-Eddy Simulation Model for Numerical Investigation of Wall-Bounded Turbulent Flows. AIAA-2022-3328, 2022.

Other Significant Products, Whether or Not Related to the Proposed Project (see PAPPG Chapter II.D.2.h.i.a.5)

6. Ranjan, R., Pantano, C., & Fischer, P. (2010). Direct simulation of turbulent swept flow over a wire in a channel. Journal of Fluid Mechanics, 651, 165-209.

7. Ranjan, R., & Pantano, C. (2013). A collocated method for the incompressible Navier–Stokes equations inspired by the Box scheme. Journal of Computational Physics, 232(1), 346-382.

8. Ranjan, R., Muralidharan, B., Nagaoka, Y., & Menon, S. (2016). Subgrid-scale modeling of reaction-diffusion and scalar transport in turbulent premixed flames. Combustion Science and Technology, 188(9), 1496-1537.

9. Ranjan, R. (2020). Integral length-scale approximation based modeling of subfilter-scale scalar flux for large-eddy simulation of stratified turbulent flows. In APS Division of Fluid Dynamics Meeting Abstracts (pp. R07-006).

10. Ranjan, R., & Menon, S. (2021). Two level simulation of Schmidt number effect on passive scalar transport in wall-bounded turbulent flows. Physics of Fluids, 33(3), 035124.

***Synergistic Activities - (see PAPPG Chapter II.D.2.h.(i)(a)(6))**

1. The investigator has worked on the development and application of high-fidelity numerical approaches, which has led to solvers such as BoxNS (a parallel incompressible flow solver with discretely mimetic properties) and CoolSim (a state-of-the-art tool for investigation of flow and heat transfer in data-center facilities). In addition, the investigator has worked on the continued development focused on novel modeling capabilities, modernization, and management of flow solvers such as in-house version of OpenFOAM, AVF-LESLIE (a combustion simulation code), and MINCLES (an incompressible flow solver with multi-scale modeling capabilities).

2. The investigator was involved in the development and modernization of AVF-LESLIE, a combustion simulation code, which reached a milestone for in situ visualizations to achieve “extreme scale knowledge discovery”. The accomplishment was credited to the expertise of the collaborators, which included Intelligent Light Inc., Georgia Tech and Lawrence Berkeley National Laboratory with funding from the Department of Energy.

3. The investigator has chaired sessions at several different conferences and student competitions. The investigator chaired the CFD topic of the AIAA Aviation 2024 and is a senior member of the AIAA’s Fluid Dynamics Technical Committee.

4. The investigator has mentored 2 high-school students, 2 UT Promise scholars, 2 UTC’s Honors College students, 25 undergraduate students, 14 graduate students in their thesis research, and advised/ co-advised 10 graduate students.

5. The investigator has established and is using several collaborative and documentation strategies by using TRAC and Sphinx tools for efficient transfer of knowledge to students, development of databases, and establishment of best practices.

***Certification**:

When the individual signs the certification on behalf of themselves, they are certifying that the information is current, accurate, and complete. This includes, but is not limited to, information related to domestic and foreign appointments and positions. Misrepresentations and/or omissions may be subject to prosecution and liability pursuant to, but not limited to, 18 U.S.C. §§287, 1001, 1031 and 31 U.S.C. §§3729-3733 and 3802.

Signature (Please type out full name): Reetesh Ranjan Date: 7/25/2023

Biographical Sketch

Sungwoo Yang
University of Tennessee at Chattanooga
Department of Civil and Chemical Engineering
Phone: 423-425-4366 Fax: 423-425-5229 Email: Sungwoo-yang@utc.edu

(a) Professional Preparation

Undergraduate	Ajou Univ. & IIT	Chemical Engineering	B.S. 2006
Graduate	Duke University	Chemistry	Ph.D. 2011

(b) Appointments

2012 – 2017 Massachusetts Institute of Technology (MIT), Research Scientist
2017 – Present University of Tennessee at Chattanooga, Assistant Professor

(c) Publications

(i) Most Closely Related Products

1. L Zhao, B Bhatia, S Yang, E Strobach, LA Weinstein, TA Cooper, EN Wang, Harnessing Heat Beyond 200° C from Unconcentrated Sunlight with Non-Evacuated Transparent Aerogels, ACS Nano, **2019**, 13 (7), 7508
2. E Strobach, B Bhatia, S Yang, L Zhao, EN Wang, High temperature stability of transparent silica aerogels for solar thermal applications, APL Materials, **2019**, 7 (8), 081104
3. L Zhao, E Strobach, B Bhatia, S Yang, A Leroy, L Zhang, EN Wang, Theoretical and experimental investigation of haze in transparent aerogels, Optics express, **2019**, 27 (4), A39-A50
4. LA Weinstein, K McEnaney, E Strobach, S Yang, Hybrid Electric and Thermal Solar Receiver, *Joule*, 2 (5) **2018**, 962-975A
5. E Strobach, B Bhatia, S Yang, L Zhao, EN Wang, High temperature annealing for structural optimization of silica aerogels in solar thermal applications, *Journal of Non-Crystalline Solids*, **2017**, 462, 72-77
6. Yang, S., Huang, X., Chen, G. et al. Three-dimensional graphene enhanced heat conduction of porous crystals, *J Porous Mater* (**2016**) 23: 1647
7. L Zhao, S Yang, B Bhatia, E Strobach, and EN. Wang, Modeling silica aerogel optical performance by determining its radiative properties, *AIP Advances* 6, 025123 (**2016**)

(ii) Other Products

1. H. Kim, S. Yang, S. Narayanan, H. Furukawa, J. Jiang, A. Umans, O. Yaghi and E. Wang, Harvesting Water from Humid Air using Metal-Organic Frameworks, Science 356, 6336, 430-434 (2017)
2. H Kim, SR Rao, EA Kapustin, L Zhao, S Yang, OM Yaghi, EN Wang, Adsorption-based atmospheric water harvesting device for arid climates, Nature communications 9 (1), 1191 (2018)
3. S. Yang, H. Kim, S. Narayanan, I. McKay and E. Wang, Carbon Nanomaterials as Binders for Advanced Thermal Batteries, Materials & Design 2015, 85, 520
4. S. Narayanan, H. Kim, A. Umans, S. Yang, X. Li, S. Schiffres, S. Rao, C. Rios, C. Hidrovo, and E. Wang, A Thermophysical Battery for Storage-based Climate Control, Applied Energy, 189, 1, 31–43 (2017)
5. A Rieth, S Yang, E Wang, M Dinca, Record Atmospheric Fresh Water Capture

and Heat Transfer with a Material Operating at the Water Uptake Reversibility Limit, ACS Cent. Sci., 3 (6), pp 668–672 (2017)
6. H. Kim, H. J. Cho, S. Narayanan, S. Yang, S. Schiffres, X. Li, H. Furukawa, Y. Zhang, J. Jiang, O. M. Yaghi and E. N. Wang, Characterization of Adsorption Enthalpy of Novel Water-Stable Zeolites and Metal-Organic-Frameworks, Scientific Reports, 2016, 6, 19097
7. S. Narayanan, X. Li, S. Yang, H. Kim, A. Umans, I.S. McKay, E.N. Wang, Thermal battery for portable climate control, Applied Energy, 149, 104-116, 2015.
8. S. Narayanan, S. Yang, H. Kim, and E. Wang, Optimization of Adsorption Processes for Climate Control and Thermal Energy Storage, Journal of heat transfer, 2014, 77, 288–300.

(d) Synergistic Activities

- **Interdisciplinary research approach.** The focus of Dr. Yang's research is on porous materials which intersect the multidisciplinary fields of solar energy harvesting and thermal energy storage. He has been collaborating with multiple faculties in Mechanical Engineering and Chemistry Departments as well as UTC's SimCenter.
- **Local industry collaboration**. Dr. Yang has been working with The Hamilton County Water & Wastewater Treatment Authority (WWTA) as the community partner for partnership and potential for joining funding.

NAME: Morgan F. Smith

POSITION TITLE & INSTITUTION: Assistant Professor, University of Tennessee, Chattanooga

A. PROFESSIONAL PREPARATION - (see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
University of West Florida	Pensacola, Florida	Anthropology	BA	2013
Texas A&M University	College Station, Texas	Anthropology	PhD	2019

B. APPOINTMENTS - (see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
2019-Present	Assistant Professor, Department of Social, Cultural, and Justice Studies, University of Tennessee, Chattanooga
2021-Present	Courtesy Assistant Professor, Department of Anthropology, Florida State University, Tallahassee, Florida
2013-2019	Graduate Assistant Lecturer, Anthropology Department, Texas A&M University, College Station, Texas.
2010-2019	Archeological Technician, Southeast Archeological Center, National Park Service, Tallahassee, Florida.

C. PRODUCTS - (see PAPPG Chapter II.C.2.f.(i)(c)) Products Most Closely Related to the Proposed Project

2021- "A Reexamination of the Alexon Bison Site, Florida." By Michael R. Waters, Zachary N. Newall, and Morgan F. Smith. PaleoAmerica, 7:3, 280-285.

2021- "The magnificent seven: Marine submerged precontact sites found by systematic geoarchaeology in the Americas." By Michael K. Faught and Morgan F. Smith. Published in the Journal of Island and Coastal Archaeology, 16:1 86-102.

2021- "Acoustic Mapping of Submerged Stone Age Sites—A HALD Approach." By Ole Grøn, Lars O. Boldreel, Morgan F. Smith, Shawn Joy, Rostand Tayong Boumda, Andreas Mäder, Niels Bleicher, Bo Madsen, Deborah Cvikel, Björn Nilsson, Arne Sjöström, Ehud Galili, Egon Nørmark, Changqing Hu, Qunyan Ren, Phillipe Blondel, Xing Gao, Petra Stråkendal, and Antonio Dell'Anno. Remote Sensing, 13(3): 445.

2020- "Site Formation Processes and Geoarchaeology at the Ryan-Harley Site, Florida, USA." By Morgan F. Smith. Geoarchaeology, 2020; 35: 451– 466.

2019- "Hunting an Underwater Mammoth: A Re-Evaluation of the First Submerged Prehistoric Site Excavated in the Americas." By Morgan F. Smith. In "New Directions in the Search for the First Floridians" ed. David Thulman and Ervan Garrison. University of Florida Press.

Other Significant Products, Whether or Not Related to the Proposed Project

2020- “FSPLASH: A Review of 2019 and 2020 Activities.” Morgan F. Smith and Shawn Joy. Submitted to the Florida Division of Historical Resources and Florida Bureau of Archaeology Research, 8/10/2020.

2019- “Emerging Remote Sensing Methods in Underwater Archaeology.” Tim DeSmet and Morgan F. Smith. In “New Directions in the Search for the First Floridians” ed. Dave Thulman and Ervan Garrison. University of Florida Press.

2019- "Analysis of a coprolite from Conejo Shelter, Texas: Potential ritualistic Viperous snake consumption." Elanor Sonderman, Crystal Dozier, and Morgan F. Smith. Journal of Archaeological Science: Reports 25, 85-93.

2018- “Submerged,” in the Active Archaeology Notebook, pp 19-21. Thames and Hudson. Edited by Leah McCurdy. A classroom exercise in underwater archaeology.

2018- “pHreservation,” in the Active Archaeology Notebook, pp 31-35. Thames and Hudson. Edited by Leah McCurdy. A classroom exercise in geoarchaeology.

D. SYNERGISTIC ACTIVITIES - (see PAPPG Chapter II.C.2.f.(i)(d))

I am partnered with the Center of Excellence for Applied Computational Science and Engineering in Chattanooga, TN, to advance theoretical acoustic studies and geophysical modeling at the University of Tennessee, Chattanooga.

I am partnered with Upward Bound Math/Science in Chattanooga, TN to teach archaeological science to high schoolers with disadvantaged socioeconomic backgrounds.

I am currently partnering with the Florida Fish and Wildlife Conservation Commission (FW) to increase knowledge of FWC officials regarding underwater archaeological sites.

I organized four separate field projects in 2018, 2019, and 2021 aimed specifically at training undergraduate and graduate students from five universities (two of which are international) on underwater geophysical methods, including side-scan and sub-bottom SONAR.

I am partnering with the Southeast Climbers Coalition (SCC) and the Eastern Band of the Cherokee Indian to survey lands owned by the SCC for culturally significant resources.

Boris P Belinskiy
UC Foundation Professor | Department of Mathematics
University of Tennessee at Chattanooga | Chattanooga, TN 374-3-2598
Tel: 423-425-4748, Email: Boris-Belinskiy@utc.edu

A. Professional Preparation:

St. Petersburg University	Mathematical Physics	BS	1968
St. Petersburg University	Mathematical Physics	MS	1970
St. Petersburg University	Mathematics	PhD	1972
St. Petersburg University	Mathematics	DSc – 2nd Doctoral Degree	1986

B. Appointments:

1998 - pres. Professor
Department of Math., University of Tennessee at Chattanooga
1997 - pres. Univ. of Tennessee Foundation Professor
1996 - 1997 Univ. of Chattanooga Foundation Associate Professor
1995 - 1996 Associate Professor
1994 - 1995 Assistant Professor
1993 - 1994 Visiting Instructor
Department of Math. & Statistics, Univ. of North Florida
1992 - 1993 Adjunct Faculty
Department of Math. & Statistics, Univ. of North Florida
1987 - 1991 Leading Research Scientist
Department of Math & Mathematical Physics, St. Petersburg Univ., Russia
1976 - 1987 Senior Research Scientist
Department of Math & Mathematical Physics, St. Petersburg Univ., Russia
1973 - 1975 Research Scientist
Department of Math & Mathematical Physics, St. Petersburg Univ., Russia

C. Selected Recent Publications

Five publications most closely related to proposed project:

- Optimal design of a fin in steady state (with J. W. Hiestand and L. Weerasena), Appl. Mathem. Model., 77, Part 2, 1188-1200, 2020.
- Optimal Effectiveness and Efficiency of a Fin in Steady-State: Multi-objective Approach (with J. W. Hiestand and L. Weerasena), Optimization and Engineering, 1-24 (April), 2020.
- Stefan-Boltzmann Problem for Heat Transfer in a Fin (with J. Graef and L. Kong), Math Meth Appl Sci. 44, 4745-4755, 2021.
- Singular Sturm--Liouville operators with extreme properties that generate black holes (with D. Hinton and R. Nicholas), Stud Appl Math, 1-29, 2021,

- Optimal design of minimum mass structures for a generalized Sturm-Liouville problem on an interval and a metric graph (with D. H. Kotval), Electron. J. Differential Equations, Vol. 2018, No. 119, pp. 1-18, 2018.

Five other significant publications:

- Time optimization of a draining tank and some similar problems on star graphs (with D. C. White), Punjab Univ. J. of Math, Vol. 51(7), 1-18, 2019.
- On the parabolic equation method for the problem of diffraction by strongly elongated spheroid (with I. V. Andronov), J. of Math Analysis and Applications, Vol. 456, Issue 2, 1176-1202, 2017.
- Piecewise uniform optimal design of a bar with an attached mass (with J. V. Matthews and J.W. Hiestand), Electron. J. Diff. Equ., 2015, 1-17, 2015.
- On Controllability of a Non-homogeneous Elastic String with Memory (with S. A. Avdonin), J. of Math Analysis and Applications, 398, 254-269, 2013.
- Optimal Design of a Bar with an Attached Mass for Maximizing the Heat Transfer (with James W. Hiestand and Maeve L. McCarthy), Electron. J. Diff. Equations, Vol. 2012, No. 181, pp. 1-13, 2012.

D. **Synergistic Activities**:

- Thesis advisor for 1 PhD student and several MS students (St. Petersburg University)
- Thesis Advisor for one Undergraduate Honor Student, one MS Student, and 2 PhD students (University of Tennessee at Chattanooga)
- Committee member for several MS and PhD students (University of Tennessee at Chattanooga)
- Organizer of several special sessions and one conferences on Applied Mathematics

NSF BIOGRAPHICAL SKETCH

NAME: Dr. Lan Gao

POSITION TITLE & INSTITUTION: Professor of Statistics, The University of Tennessee at Chattanooga

A. PROFESSIONAL PREPARATION

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
Wuhan Textile University	Wuhan, PRC	Textile Engineering	BS	1996-2000
University of Mississippi	Oxford, MS	Statistics	Ph.D.	2005-2010
St Jude Children's Research Hospital	Oxford, MS	Postdoc training in Biostatistics		2010-2012

B. APPOINTMENTS

From - To	Position Title, Organization and Location
2023-present	Professor, Department of Mathematics, University of Tennessee at Chattanooga
8/2017-7/202	Associate Professor, Dept. of Mathematics, University of Tennessee at Chattanooga
8/2012-7/2017	Assistant Professor, Dept. of Mathematics, University of Tennessee at Chattanooga
2014-Present	Biostatistics Faculty, The University of Tennessee College of Medicine at Chattanooga

C. PRODUCTS

Products Most Closely Related to the Proposed Project

1. Jacob and L. Gao et. al. "Vascular Comorbidities Worsen Prognosis of Patients with Heart Failure Hospitalized with COVID-19" BMJ Openheart Vol.8 Issue 1, 2021.

2. Theresa Sevilis and L. Gao et. al. "Telestroke: Maintaining Quality Acute Stroke Care during the COVID-19 Pandemic", Telemedicine and E-health, https://doi.org/10.1089/tmj.2021.0149.

3. Manish Tripathi and C. Gao et al., "Z Probe, an Efficient Tool for Characterizing Long Non-Coding RNA in FFPE Tissues", Journal of Non-Coding RNA, Special Issue 4-20, 2018.

4. L. Zhu, S. Pounds, L. Gao and R. Gilbertson et al., "Multi-organ mapping of cancer risk", Cell, 166 (5):1132-1146, 2016.

5. D. Kawauchi and L. Gao and etc. "A mouse model for the most aggressive molecule subtype of human Medulloblastoma", Cancer Cell, vol. 21 (2), pp. 168-180, 2012.

Other Significant Products, Whether or Not Related to the Proposed Project

1. L. Gao and B. ShC. Murphy, B. Foster, "Temporal Dynamics in Rhizosphere Bacterial Communities of Three Perennial Grassland Species", Multidisciplinary Digital Publishing Institute Agronomy 2016, 6, 17.
2. L. Gao and C. Cheng, "A phenotype-drive dimension reduction (PhDDR) approach to integrated genomic association analysis", IEEE Engineering in medicine and Biology Society, pp.6837-40(2011).
3. S. Pounds, L. Gao, R. Johnson, K. Wright, H. Poppleton, D. Finkelstein, S. Leary and R. Gilbertson, "A procedure to statistically evaluate agreement of differential expression for cross-species genomics", Bioinformatics, 27 (15), pp.2098-2103 (2011).

D. SYNERGISTIC ACTIVITIES

Most recently Gao was awarded the Biomedical Initial Collaborative Research grant for academic year of 2020 as PI of UTC campus.. She designed clinical experiments, develop statistics methods and conduct statistics analysis to investigate the association between hyperchloremia and in-hospital mortality among critically ill adult patients. Gao is currently investigating NSF founded program HDR DHC Collaborative Research (2019-2022) on data science as Co-PI. The major goal of this NSF project program is to train undergraduate and graduate students with strong interdisciplinary knowledge and skills, and provide them with new education and research experiences that will promote their career development in the data science fields. The program encompasses a breadth of applied and computational mathematics, statistics, business, computer science. Dr. Gao takes a leadership role to train undergraduate students in data analytics and simulations studies using statistical models.

NAME: Nagwan R. Zahry

POSITION TITLE & INSTITUTION: Assistant Professor-University of Tennessee at Chattanooga

A. PROFESSIONAL PREPARATION
(see PAPPG Chapter II.C.2.f.(i)(a))

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
American University in Cairo	Cairo, Egypt	Communication	BA	2004
American University in Cairo	Cairo, Egypt	Political Science	MA	2008
Michigan State University	East Lansing, Michigan	Media and Information	PhD	2017

B. APPOINTMENTS
(see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
2018-Present	Assistant Professor, University of Tennessee-Chattanooga, Chattanooga, TN
2017 - 2018	Assistant Professor, Michigan State University, East Lansing, MI
2017 – 2018	Research Project Manager, Michigan State University, East Lansing, MI
2012 - 2017	Research Assistant, Michigan State University, East Lansing, MI
2009 - 2012	Program Manager, MUCIA [Midwest Universities Consortium for International Activities (including universities including Michigan State University, the Ohio State University, University of Illinois, University of Minnesota, Purdue university, and Iowa State University], Cairo, Egypt - USA
1995 - 2008	Communication Manager, Financial Services Project – Funded by United States Agency for International Development (USAID), Cairo, Egypt.

C. PRODUCTS
(see PAPPG Chapter II.C.2.f.(i)(c))
Products Most Closely Related to the Proposed Project

1- Zahry, N. & Besley J.C. (2021). University attendance as science communication. International Journal of Science Education, Part B. 11(2):155-173.
2- Zahry, N. & Besley, J.C. (2021). Can scientists communicate interpersonal warmth? Testing warmth messages in the context of science communication. Journal of Applied Communication Research, 1-19.
3- Besley J.C., Zahry, N.R., McCright, A., Elliott K., Martin, J., & Kaminski N. (2018). Conflict of Interest Mitigation Procedures May Have Little Influence on the Perceived Procedural Fairness of Risk-Related Research. Risk Analysis, 1-15.
4-Besley, J.C., McCright, A. Zahry, N.R., Elliott, K., Martin, J., Kaminski, N., (2017). Perceived Conflict of Interest as Procedural Fairness in Health Science Partnerships. PLOS ONE, 1-20.
5- Zahry, N., & Besley, J.C. (2017). Genetic engineering, genetic modification, or agricultural biotechnology: does the term matter? Journal of Risk Research, 22(1):16-31.

Other Significant Products, Whether or Not Related to the Proposed Project

1- Ling, J., Zahry, N., & Liu, C. (2021). Stress management interventions among socioeconomically disadvantaged parents: A meta-analysis and moderation analysis International Journal of Nursing Studies,120:103954.
2- Zahry, N, Besley J.C. (2019). Warmth portrayals to recruit students into science majors. Visual Communication, 1470357219871696
3- Zahry, N.R. & Ling, Y. (2019). Parental Perceived Facilitators for and Barriers to Participating in Lifestyle Interventions to Reduce Early Childhood Obesity. A Qualitative Evaluation. Western Journal of Nursing Research, 0193945919866691
4- Zahry, N.R., Cheng, Y., & Peng, W. (2016). Content Analysis of Diet-Related Mobile Apps: A Self-Regulation Perspective. Health Communication, 1-10.

D. SYNERGISTIC ACTIVITIES
(see PAPPG Chapter II.C.2.f.(i)(d))

1- Using a phenomenological data analysis approach, I examine the effect of the COVID-19 on low-income families lifestyle behaviors.
2- Pediatric Overweight and Obesity Prevention. In collaboration with faculty in the College of Nursing at Michigan State University, I examined the effect of lifestyle interventions on low income parents an preschoolers
3- Eating Behavior and Technology. Based on examining 400 mobile application using Social Cognitive Theory, my research show diet-related apps include selfi--monitoring, rewards adn social comparison can help consumes regular unhealthy eating.
4- Science Communication and Food Labeling. My research shows that framing GMO products usign term such as "Agricultural biotech" can positively affect consumers' buying behaviors.
5- Increase understanding of science related topics. I focus on counteracting negative stereotypes of scientists.

Appendix B

Awardee Project Reports
FY 2023

Fiscal Year 2023 Annual Project Report –

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Dr. Sandra C. Affare, Lead PI

Co-PI(s): N/A

Other Personnel: N/A

Project Title: "Food Desert Identification and Elimination System"

Date Submitted: April 30, 2023

Award Start – End Date: July 1, 2022 – March 31, 2023

Non-Technical Summary:

The purpose of this computational science and engineering project is to develop a web application to support the identification of local areas greatly impacted by limited access to fresh fruit and vegetables. The project's outcome is a food desert identification and elimination system prototype. Application of this developed system will foster the development of technology-savvy youth who can solve a real-world problem of limited access to fruit and vegetables in food deserts using computational modeling and simulation. This project built a computational/GIS prototype with a front-end interface that will be used to better identify, characterize, and remediate food deserts. If successfully implemented, the developed prototype can make significant impacts on food desert research and provide a transformative field-based educational model.

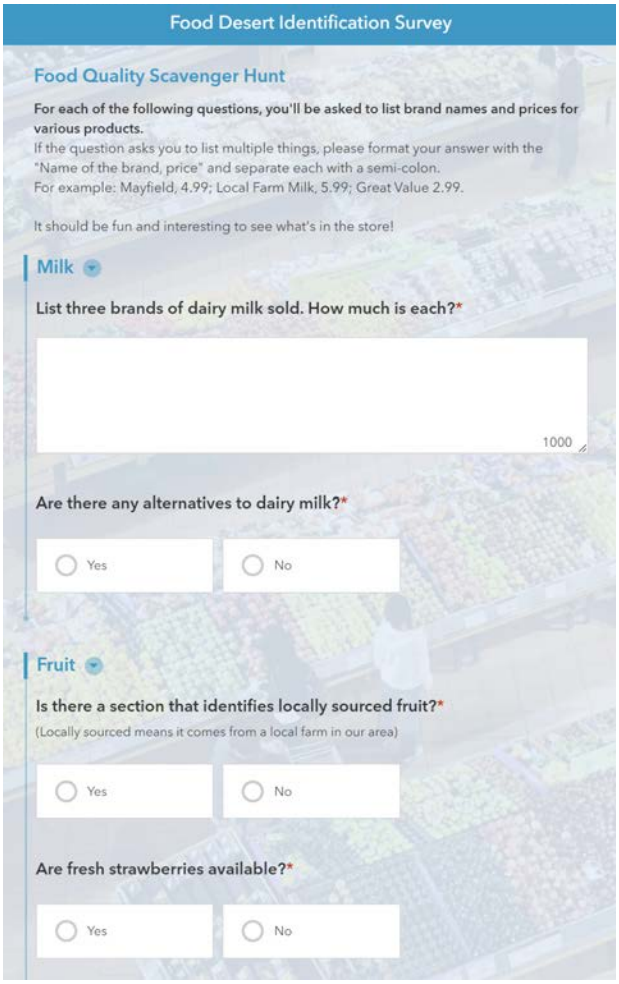
The project produced a conference presentation, provided a collaborative opportunity with an existing externally funded STEM-education program for minority females, and supported an opportunity to seek additional external funding. Two undergraduate students worked on this project. One student has received an internship that can lead to employment upon graduation in December 2023. This project expands support beyond the University and contributes to the SimCenter's mission by introducing modeling and simulation to a middle school audience.

PROJECT TITLE: "Food Desert Identification and Elimination System"

Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
This web application will help raise awareness of food access problems.	The project's outcome is a food desert identification and elimination system prototype.

RESULTS



OTHER INFO

Budget and Schedule

Total Budget:	$15,991.00
Actual Used:	$14,082.42
Balance:	$ 1,908.58

Total period of performance is 12 months.

Task 1: Understanding information needed to develop the Data Layer.
Task 2: Identifying the Service Layer
Task 3: Developing the System Front-End (Web Application)

Deliverables

- Mid-Year and Final report detailing results, financials, and milestones completed.
- Internal conference presentation (Research Dialogues)

Organization Information

Engineering Management & Technology
615 McCallie Avenue, Dept.
Chattanooga, Tennessee 37403

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The purpose of this computational science and engineering project is to develop a web application to support the identification of local areas greatly impacted by limited access to fresh fruit and vegetables. This web application will provide an opportunity to raise awareness of food access problems and promote computational science and engineering to the public, especially to underdeveloped and underrepresented groups. The web application serves as a presentation layer to users, which accepts user queries, sends processing tasks to the server, and then renders server results. For instance, the user can map all food deserts near a location he/she chooses with this application and plot future locations of food pantries.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
This project proposed to build a computational/ GIS model with a front-end interface that will be used to better identify, characterize, and remediate food deserts.	The project was successful in completing the front-end interface that will be used to collect food desert data that will be used to better identify, characterize, and remediate food deserts. [See Survey 1,2,3 interface on previous page.] All the collected data will be preprocessed to form usable datasets for later food desert projects.

Challenges & Strategies Used to Address / Overcome:

The undergraduate engineering students hired were not familiar enough with the ArcGIS tools to design and develop the web-based interface. This provided a longer learning curve in getting them trained and up to speed to perform the work presented in the proposal. The PI pivoted quickly and assigned them a smaller part of the project which gave them a win (in two months) and developed their confidence to complete the larger tasks.

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

The PI realized during the proposal stage that all work could not be completed in one year and therefore planned to incorporate the outcomes in the USDA Award.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

Participation in the CEACSE proposal process provided significant growth, strategic multi-disciplinary partnerships across UTC's campus, and opportunities to excel in my research. The useful feedback from the proposal submission improved the PIs ability to write future proposals and their potential for meaningful follow-on extramural funding. As an Adjunct, there are extremely

limited opportunities to lead academic research. This Mini CEACSE grant provided the PI an opportunity to lead academic research.

This project produced a solid collaboration between the PI and UTC's Interdisciplinary Geospatial Technology (IGT) Lab managers. They provided GIS and technical management and direction to the students to create the food desert maps using spatial analysis and spatial data science methods. IGT Lab's access to Community and Business analyst resources (demographic/ socioeconomic information) from Esri's Living Atlas at the census block level was extremely helpful in creating these maps. IGT Lab's Desktop and SaaS (Cloud) resources were utilized for processing, analysis, storage, cartography, and the development of focused GIS web applications and maps for final analysis results sharing. It is anticipated that this smooth experience will result in future proposal collaborations, presentations, and publications.

Students Impacted

Dexter Digby: Mr. Digby is a Senior Engineering Management and Technology undergraduate student who is scheduled to graduate in December 2023. The student worked on the project during the Fall 2022 semester and received an internship with the Electric Power Board beginning in the Spring of 2023. During the Mid Term Status meeting, Mr. Digby presented a working prototype of the web-based tool that will be used to collect data and document food access and food security concerns.

Markintus Morris: Mr. Morris is a Computer Science and Engineering Management undergraduate student. He worked on the project for less than two months in the Spring of 2023.

Community and Broader Impacts

The United States Department of Agriculture (USDA) defines a ***food desert*** as an area where people live more than a mile from the nearest grocery store in urban areas. In food deserts, there is limited access to fresh fruit, vegetables, and other whole foods. The Hamilton County Health Department reports more than 32,000 people in Hamilton County living in areas that are considered food deserts. In 2019, there were fourteen tracts of land within Hamilton County, which qualify as food deserts (Howell, 2019).

To address the identified food deserts, as a result of the prototype developed with this funding, participants in the collaborative ANGELS program will be able to collect food desert data and simulate placements of food pantries. A project-based learning approach will provide a unique environment for participants to identify food deserts using geospatial information and data analytics methods, examine the evidence, ask questions, then propose solutions to the problem. The geospatial information not only aims to identify food desert using the tools, but also provides hands-on training of the technology to middle school females, which could make a broader policy and educational impact.

After using technology to identify the areas, data integration and normalization will assist the students in forming and evaluating their hypotheses to deliver innovative solutions. This agricultural experiential learning and non-traditional educational opportunity helps create a successful middle school to college pathway leading to STEM-related careers. The middle school

female students represent a diverse community of learners who will contribute to a knowledgeable, future workforce. If the model and interface could be generalized to other cities, it could be useful in addressing food deserts elsewhere.

Scholarly Product

Presentation at UTC:

- Affare, S. and Hunt, N. "Food Desert Identification and Elimination System." UTC Spring Research and Arts Conference. (Non-Refereed Conference), April 2023.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

This work resulted in a ***continued*** collaboration with Dr. Jose Barbosa, a full professor in the Biology, Geology and Environmental Science Department. Dr. Barbosa is interested in continuing food desert research that will help identify and eliminate food deserts through community gardens. He is willing to share his gardening expertise with underserved communities.

EXTERNAL FUNDING

Proposal Submission

- Barbosa, J., Kaplanoglu, E., **Affare, S.** and Zahry, N. "Community-Driven Approach to Food Desert Elimination with STEM-Education & Agricultural Projects" (Agriculture and Food Research Initiative Competitive Grants Program Education and Workforce Development Program Grant submitted March 2023) **$627,426** – *pending.*

Contracts/Awards Received

While the following program was submitted prior to the reporting period, it is immediately related to the awarded CEACSE Mini Grant work.

- "Agriculture and Nutrition for Girls while Encouraging Leadership & STEM-Enrichment" (ANGELS) (submitted to USDA for Women and Minorities in STEM (WAMS) Program Grant, March 2022) Role: Co-PD (PD: Dr. José M. Barbosa) Awarded: **$99,561**

Sponsored Program Capacity Building Activities

- Participated in a National Science Foundation (NSF) Panel – 2022
- NSF STEM PEER Academy Fellow 2022 - 2023
- NSF grant webinars
- Attended UTC Promotion & Tenure Workshop

PLAN FOR COMPLETION DURING THE NEXT FISCAL YEAR (EXTENSION PERIOD)

The web application prototype developed as a result of this grant award will be tested and evaluated during the ANGELS Summer Pilot (June - July 2023) and the ANGELS Enrichment Program (2023-2024 Hamilton County School Year). The ANGELS Programs are supported by the United States Department of Agriculture (USDA) National Institute of Food and Agriculture, Women and Minorities in STEM Program, Award # 2022-04279.

The data sets will be collected during the ANGELS Summer Pilot. Once datasets are ready, mathematical models can be developed to formulate food access problems and solutions. These models will be used during the ANGELS Enrichment Program to:

1) predict access to limited fresh fruit and vegetables patterns in food deserts,
2) identify potential locations for food pantries, and
3) help the ANGELS participants determine the most economic quantity of items to be stocked in those pantries.

Using spatial statistical analytics and geographic regression and machine learning cluster analysis to analyze geospatial patterns of features being mapped (geostatistical hot spots), the placement (location) of food pantries will be modeled. This will serve as an optimization problem that aims to improve access to fresh fruit and vegetables within food deserts. With the help of geographical platforms such as ArcGIS, a cross-platform, location-based application will be developed for demonstrating food pantry optimal placement. The application will allow a user to view all food deserts and household distribution in the Chattanooga area and to display the location of food proposed pantries. This web application will provide an opportunity to raise awareness of food access problems and promote computational science and engineering to the public, especially to underdeveloped and underrepresented groups.

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 in place to continue to explore the food desert research and include modeling and simulations as research and education tools in future works.

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

I would like to identify potential collaborators with medical backgrounds (medical doctors and researchers in UTC's College of Health and Human Performance) to explore the reduction of health disparities through improved access to fresh fruit and vegetables.

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

Recruiting and training undergraduate students was difficult in the time permitted. By the time they were up to speed, the planned research activities had to be shortened to ensure success. Despite this challenge, we would like to continue to support undergraduate and graduate students in research using the data that will be collected from the prototype.

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

The most significant barrier is funding availability for the PI to continue the work. As an adjunct professor, the PI has no Departmental support financially. The presents competing time priorities for other paid activities.

FINANCIAL ACCOUNTING

The PI requested an additional $1,000 to be added to the Budget to cover the project's spending projections for the last quarter. The funds that were projected for IGT Lab Managers were not spent; one manager was on extended leave during the project's period and in the end did not have remaining supervision charges due to a student worker's time ending. One student had a heavy courseload, limiting their ability to put more into the project in the last quarter.

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Murat Barisik, Lead PI

Project Title: "Molecular Modeling of Electric Double Layer and Nanoscale Heat Transfer in Supercapacitors"

Date Submitted: 07/01/2022

Award Start – End Date: July 1, 2022 – June 30, 2023

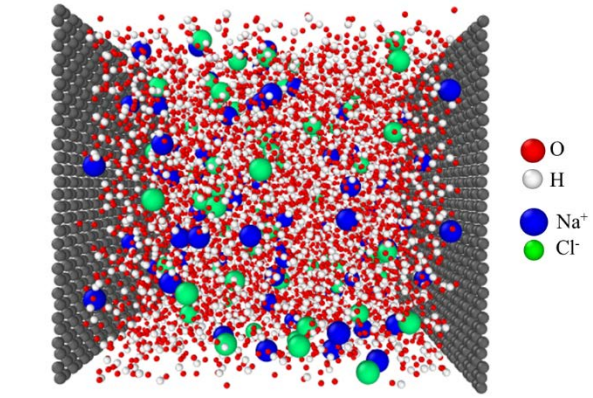
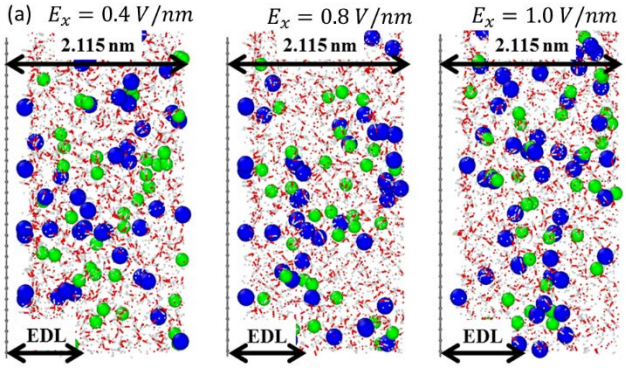
Non-Technical Summary:

The US Department of Energy (DOE) suggests that the need for energy storage is expected to grow substantially in the coming years. Recent energy storage and conversion applications require a thorough knowledge of the behavior of electrode/electrolyte interfaces. However, electric double layer (EDL) formation through an electrolyte is not well understood yet. Both ionic layering and heat transfer behavior show non-continuum behavior as the molecular level mechanisms become dominant in EDL. For such a case, I developed Molecular Dynamics modelling of ionic solutions confined in nanoscale graphene channels. Through this project, I obtained the ability to molecularly simulate solid graphene, water and NaCl solution, and electric double layer formation under different salt and electric field conditions. I presented the current idea and the preliminary findings at Oak Ridge National Laborites (ORNL) as an invited seminar and at UTC Spring Research and Arts Conference. I also co-organized the "Engineering Thermal Transport in Nanoscale Materials: Recent Advances in Nanoscale Metrology and Computationally Informed Material Development" track last month in "31st International Material Research Congress" and promote my modelling capabilities. Results and abilities obtained created the founding to develop an extended proposal submitted to NSF -LEAPS-MPS program (The Launching Early-Career Academic Pathways in the Mathematical and Physical Sciences) titled as "Molecular characterization of thermal effects on capacitance behavior of supercapacitors." Currently, I am including the viscous heating mechanisms into my molecular system and revising my proposal to resubmit. As the social outreach activities, I initiated a relationship with Orchard Knob Elementary School to improve STEM education and interest in local schools. I designed a mini lesson to introduce nanoscale and related technologies to fourth grade students.

PROJECT TITLE: "Molecular Modeling of Electric Double Layer and Nanoscale Heat Transfer in Supercapacitors"

Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
Summary statement • Develop molecular model of graphene. • Develop molecular model of water. • Develop molecular model of salt solution. • Develop molecular model of electric double layer formation	I obtained the molecular model of salt solution between graphene surfaces. I observed and characterized electric double layer formation.

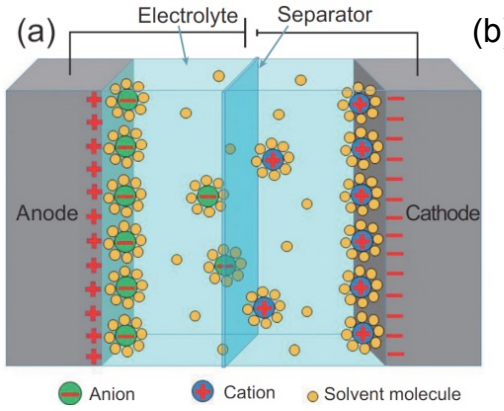
RESULTS	OTHER INFO
 	**Budget and Schedule** Total Budget: $25,000.00 Actual Used: $20,000.00 Balance: $ 5,000.00 Total period of performance is 12 months. **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication • External and internal conference presentation **Organization Information** *735 Vine St, Chattanooga, TN 37403* *murat-barisik@utc.edu*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

With the decrease in the cost of electricity generation from solar and wind power, the need for energy storage is expected to grow substantially in the coming years, as suggested by the US Department of Energy [1]. Currently, batteries are dominantly used in both large and small size applications. However, batteries have many downsides such as low power, short lifetime, low performance at low temperatures, and high fire/explosion hazard risks, so that they became the limiting factor for future technologies. In this case, ***the new generation supercapacitors (Figure 1(a)) are promising candidates for future electricity storage needs*** with light weight, fast charging, safe use and non-toxic content. The advantages of supercapacitors compared to batteries are summarized in Figure 1(b) by Maxwell Technologies company [2]. Also called double-layer capacitors, most of the supercapacitors store energy electrostatically. Different than conventional capacitors where electrodes are separated by a dielectric material, supercapacitors consist of an electrolyte solution and a separator in between two electrodes. When the electrodes are charged, ions in the electrolyte will be electrostatically attracted to the electrode surfaces which creates the so-called electric double layer (EDL). Hence, the energy is stored by the formation of this ionic layering. In the current use combined with batteries, the supercapacitors are the key to respond the variable power demands of an application since the supercapacitors can store and release short-term high powers very easily [3]. In the near future, it is expected to supercapacitors to satisfy high energy needs as well, like batteries [4]. The market size of supercapacitors showed robust growth; it reached $5.02 Billion USD value in 2021, and is expected to reach $22.50 Billion USD with a more than 4 times increase in next seven years [5].

(a)



(b)

Function	Supercapacitor	Lithium-ion (general)
Charge time	1 – 10 seconds	10 – 60 minutes
Cycle life	1 million or 30, 000h	500 and higher
Cell voltage	2.3 to 2.75V	3.6 to 3.7V
Specific energy (Wh / kg)	5 (typical)	100 – 200
Specific power (W / kg)	Upto 10, 000	1000 – 3000
Cost per Wh	$20 (typical)	$0.50 - $1.00 (large system)
Service life (in vehicle)	10 to 15 years	5 to 10 years
Charge temperature	-40 to 65^{0}C (-40 to 149^{0}F)	0 to 45^{0}C (32^0 to 113^{0}F)
Discharge temperature	-40 to 65^{0}C (-40 to 149^{0}F)	-20 to 60^{0}C (-4 to 140^{0}F)

Figure 1. (a) Schematic representation of an electrical double-layer capacitor from Ref [6], and (b) the comparison of a supercapacitor with a lithium-ion battery [3].

In order to understand the current supercapacitors and design the better ones, a thorough knowledge of the interfacial behavior between the electrode and the electrolyte is required. Specifically, ionic distribution and the resulting electric potential in the electric double layer should be resolved. In addition, thermal management of a supercapacitor should be carefully designed to control the temperature variations during the heat generation at its operation. However, ***the current literature identifies the concern of a mismatch between the theoretical estimations and the experimental observations***. Since the size of a supercapacitor is on the order of a single nanometer, the continuum descriptions are not valid to explain both ionic transport and heat transfer in such nanoscale confinement. For such a case, I developed molecular level modelling of electrode/electrolyte interfaces.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop the molecular model of multi-layer graphene system	Correct honeycomb structure and graphene stacking with correct spacing were obtained
Develop the molecular model of water	Correct water structure and thermodynamic properties were generated
Develop the molecular model of NaCl salt dissolved inside water	Correct hydrogen bond network and ion hydrations were obtained at varying ionic concentrations
Observe electric double layer formation	Correct ionic layering, electric double layer thickness, and resulting electric potential distribution were obtained

Challenges & Strategies Used to Address / Overcome:

NA

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

NA

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

By this project, I obtained fundamental molecular modelling abilities at UTC.

Students Impacted

NA

Community and Broader Impacts

Using the outcomes of this project, I will describe thermal behavior of supercapacitors which is expected to replace existing battery technologies.

I designed a mini lesson to introduce nanoscale and related technologies to local fourth grade students in the Chattanooga area.

Scholarly Products

Presentations at UTC:

- M Barisik, "Thermal Management of Electric Double-layer Capacitors for Energy Storage Applications" UTC Spring Research and Arts Conference - April 12, 2023

Inventions or Other Intellectual Property

NA

Research Outreach & Collaboration

I managed to develop close relationships with ORNL. I further developed extended proposals with my collaborators and received support from DOE.

EXTERNAL FUNDING

Proposal Submissions

- "LEAPS-MPS: Molecular characterization of thermal effects on capacitance behavior of supercapacitors" M Barisik (PI), NSF-LEAPS-MPS $250,000

Contracts/Awards Received

NA

Sponsored Program Capacity Building Activities

I attended the NSF workshop.

WHAT'S NEXT FOR THIS RESEARCH?

I will revise the proposal developed during this project. I received very positive reviews. I believe this is a very important topic for future energy technologies.

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

I will further study ionic liquids.

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

NA

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

NA

FINANCIAL ACCOUNTING

NA

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Tian Li, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: "Towards Quantum-Enhanced Bio-Sensing"

Date Submitted: June 15, 2022

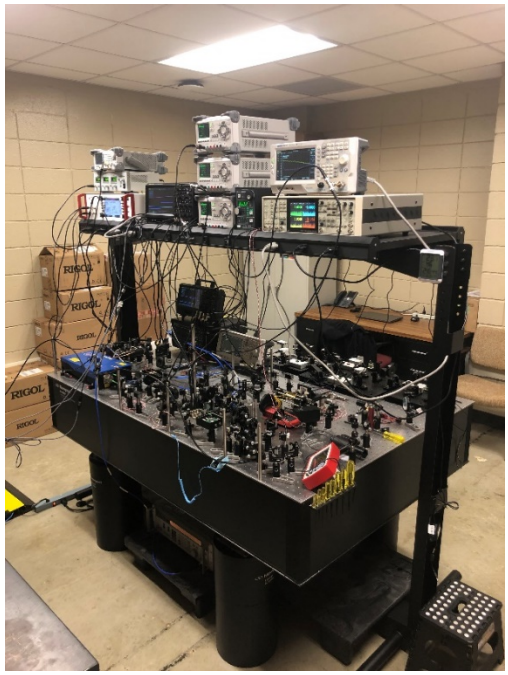
Award Start – End Date: September 1, 2022 – June 30, 2023

Non-Technical Summary:

This mini-CEACSE grant is part of the PI's offer letter's addendum. *The main purpose of this grant is to complement the PI's startup fund for establishing a quantum information science and technology (QIST) lab as stated by his offer letter's addendum*. The whole mini-CEACSE fund of $26,900 was used by the PI to purchase necessary instruments for the lab located in Grote 230. As of now, this QIST lab is fully functioning, where 70% optical noise reduction (6 dB optical squeezing, a characterization of continuous-variable quantum entanglement) is achieved on a daily basis.

The PI's ultimate goal is to utilize this continuous-variable quantum entanglement source for sensing applications, among which biological sensing is of his particular interest. Understanding biological structures and functions relies on our ability to sense and image biological molecules in their native environment, without applying any exogenous labels or modifying the system of interest. Classical sensing is very efficient down to a certain point, where stability and noise start impairing measurements. Sensing below that point (i.e., the standard quantum limit, or SQL), requires sensitivities that can only be achieved with quantum light. Both two-mode squeezed light and entangled photon pairs are ideal sources for producing super-sensitivity in metrology, as has been demonstrated with recent experiments done by the PI and his colleagues yielding 50% to 70% improvement beyond the SQL. The quantum properties of light, however, have been largely underutilized in biological spectroscopy and imaging. The PI's planned research programs at UTC aim at filling those gaps by advancing theoretical, computational, and experimental tools, which exploit quantum optical methods, nonlinear quantum spectroscopy and quantum correlations, to achieve more sensitive, chemically specific, and better resolved optical imaging of biological systems.

PROJECT TITLE: “Towards Quantum-Enhanced Bio-Sensing”
Technology Area of Interest: Health & Biological Systems + Modeling & Simulation of Quantum Systems;

TECHNICAL APPROACH	OUTCOMES
Using the fund from this mini-CEACSE grant together with the PI’s startup fund, the PI was able to purchase necessary equipment to generate continuous-variable quantum entanglement in his lab located in Grote 230, so that quantum sensing experiments using biological samples can be conducted starting Fall 2023.	A Quantum Sensing lab capable of producing 6 dB quantum squeezed light is up and running on UTC campus.
RESULTS	**OTHER INFO**
The Quantum Sensing lab is shown below: 	The total period of performance was scheduled to be 10 months (Sep.1st to Jun. 30th), however, the lase was delivered on May 15, 2023, due to supply chain backlog, thus the effective period of performance was 3 months. Total Budget: $26,900 Actual Used: $26,900 Balance: $0

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
A combined optical diagnostic and feedback system (including a Fabry-Perot cavity working as a laser spectrometer, a room temperature nature-abundant rubidium cell providing the rubidium absorption spectra, and a fiber-coupled wavemeter) for monitoring and locking the laser output at the transition of rubidium-85 D1 line at 794.9727nm	Accomplished
A double-pass acousto-optic modulator in a “cat-eye” configuration that is capable of separating the output laser beam from its input by 3.036 GHz to address the hyperfine transition in the rubidium-85 ground state	Accomplished
A homemade heat reservoir that is capable of maintaining the temperature of the rubidium-85 atomic vapor to be within ±0.2°C	Accomplished
A customized balanced photodetector with replaced photodiodes having 94% quantum efficient peaked at rubidium D1 line transition	Accomplished
Finally, a quantum light source that is capable of producing quantum entanglement in the continuous-variable regime characterized in terms of quantum noise reduction by more than 70% (i.e., more than 6 dB of squeezing)	Accomplished

Challenges & Strategies Used to Address / Overcome:

The main obstacle to the project was the delayed arrival of equipment due to the backlog of the supply chain. Some crucial instruments, such as the wavemeter for monitoring the output of the laser head and radio-frequency components for driving multiple acousto-optic modulators arrived quite late in the summer.

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

In terms of the continuous-variable quantum entanglement generation capability, everything in the PI's Quantum Sensing lab has met his expectations thus far.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

As a complement to the PI's startup fund, this mini-CEACSE grant has enabled the PI to have a substantial start on his QIST research agenda at UTC.

Students Impacted

Matthew Boone, a physics sophomore, has successfully completed his summer URP under the supervision of the PI focusing on improving the communication rate of BB84 quantum key distribution algorithm. The results of this investigation will be presented in the 90th Annual Meeting of Southeastern Section of the American Physical Society, which will be held in Eastern Kentucky University from Nov. 9th to Nov. 11th.

Community and Broader Impacts

The PI is a key member of the UTC Quantum Initiative, which is an institutional initiative with the goal to establish a program known for excellence in education, innovation, and economic development enabled by QIST. The fully functioning Quantum Sensing lab established with the help of the mini-CEACSE grant is an integral part of the initiative. The UTC Quantum Initiative is also establishing a quantum node connected to the EPB Quantum Network powered by Qubitekk and being deployed by EPB of Chattanooga. The network was announced in the 2022 Quantum World Congress and is projected to be operational by September 2023. As the PI is also in charge of the UTC quantum node lab, thus the experimental QIST research conducted in both of these two labs will naturally have broader impacts and gain more and more community exposure and as the maturing of the quantum ecosystem in the Chattanooga Metropolitan area.

Scholarly Products

Publications:

None.

External Conferences:

Matthew Boone (a physics sophomore) will present the results obtained from his summer URP project in the 90th Annual Meeting of Southeastern Section of the American Physical Society, which will be held in Eastern Kentucky University from Nov. 9th to Nov. 11th.

Presentations at UTC:

2023 Summer URP Final Presentation.

Inventions or Other Intellectual Property

None.

Research Outreach & Collaboration

1. Since joining UTC in August 2022, the PI has been collaborating with Dr. Don Reising in electrical engineering on deep-learning aided entanglement-enhanced networked sensing.
2. The PI was invited as a visiting scholar to Texas A&M University for two weeks in the summer of 2023 to conduct joint research on quantum-enhance bio-medical sensing. This is still an on-going close collaboration.
3. The PI is also collaborating with the University of North Carolina at Chapel Hill (UNC) on using quantum states of light to investigate spin dynamics in nanomagnet structures and multilayer systems involving both ferromagnetic insulators and metals.

EXTERNAL FUNDING

Proposal Submissions

1. DOE ASCR RENEW (invited)
2. DOE FAIR (invited)
3. NSF QuSeC-TAQS (2 preproposals)
4. NSF ExpandQISE (full)
5. NSF ExLENT (full)
6. NSF Engines (SEQuNA) (full)

Contracts/Awards Received

The proposal to NSF ExLENT (co-PI) has been recommended by NSF.

Sponsored Program Capacity Building Activities

The PI attended the T.I.G. group's NSF Early Career Investigators Workshop hosted by UTC's ORSP.

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 continue his experimental QIST research made possible by this mini-CEACSE for the foreseeable future.

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

Please see the "Research Outreach & Collaboration" section above for the on-going collaborations the PI has been participating in.

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?

The up-hill battle of securing external funding and gaining more visibility for UTC's quantum research and education.

FINANCIAL ACCOUNTING

None.

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Fernando Alda-Pons, Lead PI

Co-PI(s): Yu Liang
Other Personnel: N/A

Project Title: “Identification and prediction of species invasiveness potential in the gut microbiome”

Date Submitted: October 13, 2020

Award Start – End Date: July 1, 2021 – June 30, 2023

Non-Technical Summary:

Within animal digestive systems reside a vast array of microorganisms collectively known as the gut microbiome. The gut microbiome is known to play an important role in many of the host’s physiological processes, and investigating this relationship is crucial in understanding the adaptation of an animal to its environment. Species invasions offer a natural model in which to study how an abrupt change in the environment might impact the gut microbiome. We compared the gut microbiomes of four species of freshwater fish belonging to the genus Cyprinella, including both native and introduced populations of the prolific invader Cyprinella lutrensis, to investigate if differences in their diversity and structure are determined phylogenetically or depend on the ecology and geographical location where they occur.

This project has been the basis of a master’s thesis in the Department of Biology, Geology, and Environmental Science that was defended in August, 2023. The project provided funding for one graduate student and two undergraduate students. A third, undergraduate student also collaborated and participated in this project. This project has allowed the establishment of a new research line at UTC about gut microbiome and host interactions using metabarcoding technologies. Also, in the context of this new research line, we have established new collaborations with UTC faculty members. This project has resulted in novel insights about the relationships of the gut microbiome, their hosts, and the environment they inhabit. The results were presented at a local student conference at UTC and are currently under preparation to be submitted for publication in a scientific journal.

PROJECT TITLE: "IDENTIFICATION AND PREDICTION OF SPECIES INVASIVENESS POTENTIAL IN THE GUT MICROBIOME**"**
Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
• We sequenced the 16S rRNA gene V3-V4 regions to test for differences in microbial alpha diversity and community composition between species and collection sites. • We sequenced the 18S rRNA gene V9 region to test for the effects of host diet on microbial community composition.	
RESULTS	**OTHER INFO**
• A significant host effect was observed between both species and sites, and there was significant correlation between the host diet (18S) and microbial community composition. • Altogether, our results suggest that host genetics, diet, and geography all play significant roles in defining intestinal microbiota.	**Budget and Schedule** Total Budget: $90,00.00 Actual Used: $ Balance: $ 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

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Educational benefits: This project will educate and train undergraduate and graduate students on topics related to biodiversity conservation through the integration of ecology, evolutionary biology and computational sciences. Undergraduate students and graduate students will be involved in cross-campus collaborative research and will contribute to all aspects of the proposed project.	This project resulted in the completion of one master's thesis in the Environmental Science Program at BGE. Three undergraduate students participated in this project and were trained different aspects of ecology and evolutionary biology through participating in field, molecular and computational work
Institutional benefits: A key objective of the proposed work is to elevate the use of computational tools for work on biodiversity conservation, which will advance several elements (#2, #4, #5) of the UT strategic plan. The proposed project will lay the foundation for new collaborations that integrate across traditional academic disciplines, and by recruiting highly motivated and talented students into STEM programs.	This project has resulted in new collaborations with UTC faculty and in the development and establishment of a new research line at UTC.
Societal Benefits: Biological invasions are a growing anthropogenic threat to environmental and human well-being. This project will help stem the tide by providing a stronger basis for predicting and controlling invasions in aquatic ecosystems. By focusing on invasive fish in the Southeastern US, the project will also support region-wide efforts to sustain and conserve natural resources of global relevance. This will be accomplished through the development of new knowledge and tools that will generate opportunities for targeted individual-based training and public outreach and engagement on the risks and consequences of biological invasions.	There is a manuscript in an advanced stage of preparation that will be submitted shortly to a scientific journal. In this manuscript we emphasize the impact of human introductions and of biological invasions in the diversity of fish species and their gut microbiome.

Challenges & Strategies Used to Address / Overcome:

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

We found greater individual heterogeneity than expected. Ideally, we could have used a greater number of samples per species and site and/or more replicates per individual.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This project resulted in the completion of a master's thesis defended in the Department of Biology, Geology, and Environmental Science at the University of Tennessee at Chattanooga. This was the first M.S. student of the PI at UTC.

The PI established a new research line at UTC about metabarcoding and gut microbiome.

The PI also established new collaborations with other UTC faculty (Dr. Francesca Leasi).

The PI, and his student and collaborators are currently working in a scientific manuscript that will be submitted shortly for publication.

Students Impacted

The student, William Hanson-Regan was funded by this project, learned field work, molecular, and computational skills, presented his work at a local conference, and is currently in a scientific manuscript. Two undergraduate students were also funded by this project and an additional undergraduate student obtained undergraduate research credits working in this project.

William Hanson-Regan: Graduate student in the Environmental Science Program at the University of Tennessee at Chattanooga. Defended his M.Sc. Thesis in August 2023 based on the current project.

Breann Larson: Undergraduate student in Environmental Science at the University of Tennessee at Chattanooga. Was a summer student worker in this project carrying out fieldwork activities and assisting graduate student William Hanson-Regan in this project.

Joseph Watson: Undergraduate student in Biological Science at the University of Tennessee at Chattanooga. He was a summer student worker in this project carrying out fieldwork, and molecular laboratory activities to assist graduate student William Hanson-Regan in this project.

Sebastian Jimenez: Undergraduate student in Biological Science at the University of Tennessee at Chattanooga. Assisted graduate student William Hanson-Regan in this project carrying out molecular laboratory activities.

Community and Broader Impacts

Scholarly Products

Publications:

- William Hanson-Regan. Geographical, ecological, and genetic drivers of gut microbial diversity in native and invasive minnows of the genus *Cyprinella* (Actinopterygii: Leuciscidae). M.S. Thesis. University of Tennessee at Chattanooga, Chattanooga TN, USA.

Presentations at UTC:

- William Hanson-Regan, Francesca Leasi, Fernando Alda. Invasive and Native Fish Microbiomes: Identifying and Comparing the Inhabitants of Fish Guts. The UTC Spring Research and Arts Conference. University of Tennessee at Chattanooga, Chattanooga TN, USA. April 12th-13th 2023.

Inventions or Other Intellectual Property

Research Outreach & Collaboration

During the development of this project, we established new collaborations with UTC faculty Dr. Francesca Leasi, who is an expert in applying metabarcoding techniques to aquatic diversity analysis. Dr. Leasi is now a collaborator in the project, a co-author in the manuscript that is under preparation, and was a member of the graduate committee evaluating William Hanson-Regan Master's Thesis.

This project provided the framework and funding to organize and celebrate the 2nd edition of the Southeastern Computational Workshop in the SimCenter at UTC. The workshop hosted undergraduate, graduate, and faculty from five states across the nation.

EXTERNAL FUNDING

Proposal Submissions

N/A

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

- Organizer of the 2nd Southeastern Computational School in RNAseq and Transcriptome Analysis. SimCenter, University of Tennessee at Chattanooga. August 10th-12th, 2022.

WHAT'S NEXT FOR THIS RESEARCH?

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

I am no longer in academia.

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.

This work was adversely impacted by obstacles presented by the IACUC committee. In my opinion, this committee carried out parallel scientific evaluations of this project after it had been granted and evaluated by CEACSE, which delayed the onset of the project and consequently the performance of the students involved.

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

N/A

FINANCIAL ACCOUNTING

N/A

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

David Giles, Lead PI

Co-PI(s): Steven Symes and Bradley Harris
Other Personnel:

Project Title: “From in vitro to in silico: Exploring the therapeutic potential of antimicrobial peptides on exogenous fatty acid modification of bacterial membranes”

Date Submitted:

Award Start – End Date: July 1, 2022 – June 30, 2023

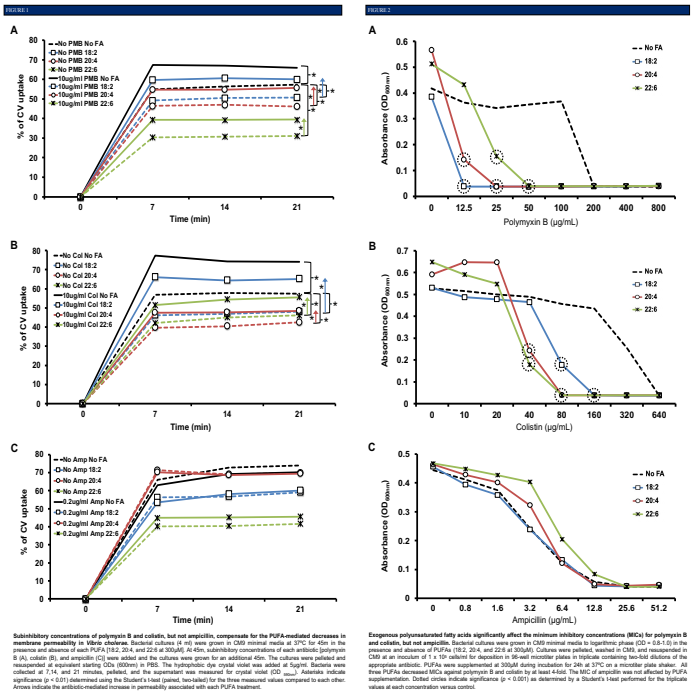
Non-Technical Summary:

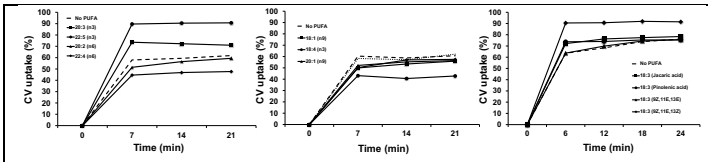
Both years of our CEACSE grant resulted in far more research successes than failures. Of the three main objectives, one proceeded exactly as planned and is in the data analysis phase. The second aim was slowed by Covid-related supply issues but is currently halfway complete with excellent results. The third aim met challenges and was adjusted to allow completion with limited time remaining for the Ph.D. student. Although not exactly as proposed, we were able to generate data that can be analyzed and interpreted for comparative value and consideration of future studies. It will be evident that the integration of computer simulations can supplement and guide in vitro studies in the field of membrane biology. This will strongly support the mission of the SimCenter.

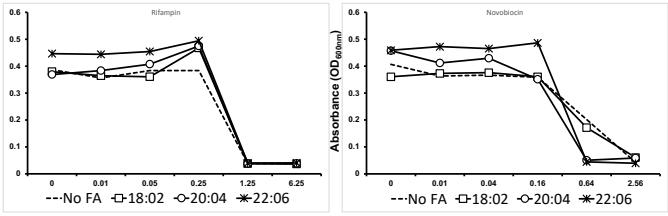
Several contributions were made by a total of 4 undergraduate students, 1 Ph.D. student, and the PIs. A total of 5 presentations (2 external and 3 internal) have been given, 1 publication was achieved, and the PI leveraged this research to obtain an additional $10,000 from a competition and was named a finalist for Early Innovator Award from a local technology council. Finally, an external NIH grant is in preparation to be submitted in the coming months. The direct training of students working on the project also indirectly affected students working in our laboratories on peripheral projects, adding to the impact of the award.

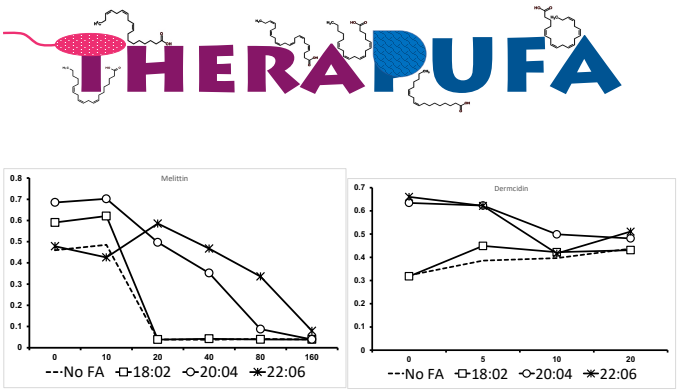
PROJECT TITLE: "From in vitro to in silico: Exploring the therapeutic potential of antimicrobial peptides on exogenous fatty acid modification of bacterial membranes"
Technology Area of Interest: Health and Biological Systems

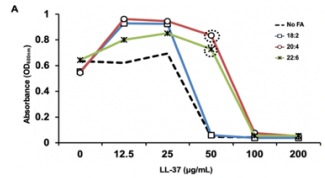
TECHNICAL APPROACH	OUTCOMES
• Quantitative Estimation of PUFA incorporation into *V. cholerae* phospholipids (Task 1) • In vitro permeability and MIC assays (Task 2) • Molecular dynamics simulations of antimicrobials (Task 3)	• *5 student presentations (3 external and 2 internal)* • *2 publications in V. cholerae (https://doi.org/10.3390/biom12091269; https://doi.org/10.1016/j.bbrep.2023.101504)* • *1 publication in closely related A. salmonicida (https://doi.org/10.1111/jfd.13715)* • *1 FLY for Researchers Competition (2nd place) [$10,000]* *Finalist for Early Innovator Award (Chattanooga Technology Council)* • *Harris Commercialization Grant [$5,000]* • *NIH R15 submitted 6/2023*

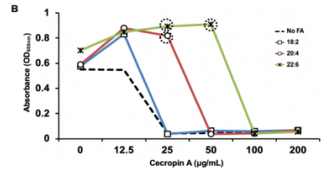
RESULTS	OTHER INFO
Include a figure as appropriate.  	*Fill in your info below.* **Budget and Schedule** Total Budget: $99,221.00 Actual Used: $99,221.00 Balance: $ 0.0 Total period of performance is 12 months. Task 1: Months 6-12 Task 2: Months 1-12 Task 3: Months 3-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved: The main development was with the UPLC/MS method for quantitation, which will be detailed in the final report. • Annual report detailing results, financials, and work plan to

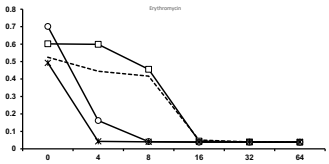


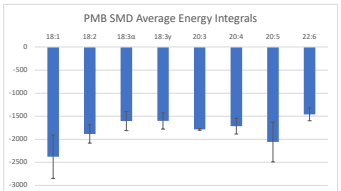


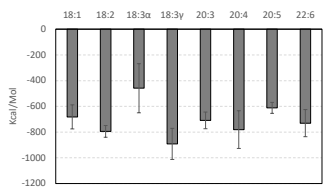


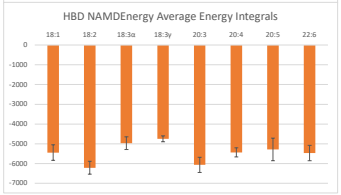


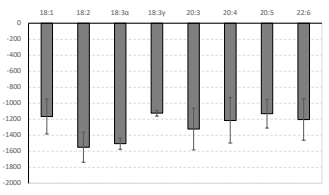












complete the project: Detailed below and in final report

- See outcomes itemized above

Organization Information

Department of Biology, Geology and Environmental Science, The University of Tennessee at Chattanooga

423-425-4341

David-giles@utc.edu

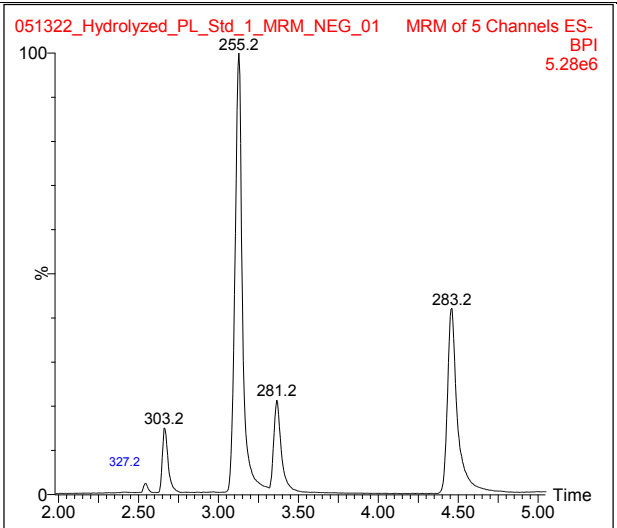


Figure 3. Fatty acids derived from hydrolysis of a test mixture of phospholipid standards (PG and PE). The sn-1 and sn-2 chains of the PLs were quantitatively cleaved and are all present in the chromatogram which elute in the following order: 22:6, 20:4, 16:0, 18:1, 18:0. Base peak m/z values in ESI- mode are indicated above each peak. Data collected by an undergraduate.

ACCOMPLISHMENTS & OUTCOMES

Project Overview

The project consisted of 3 primary objectives: 1) development of methodology to quantify the amount of exogenous fatty acid incorporation into membrane phospholipids, 2) assessment of the membrane permeability and antimicrobial resistance ramifications of PUFA/antimicrobial peptide combinations, and 3) utilization of computational modeling to generate membranes for comparison with in vitro data.

Regarding Aim 1: Our preliminary work has shown that Gram-negative bacteria are able to recognize and uptake polyunsaturated fatty acids. What is not known is to what degree PUFAs can be incorporated. We will quantify this for the first time. If a particular PUFA is found to be 100% incorporated at the 300 µM spike level, experiments will increase the spike level to determine where the degree of incorporation saturates. The prediction is that shorter FAs with fewer unsaturations will be incorporated to a higher degree than longer chains with multiple unsaturations. Our experiments will be designed to test this.

To determine the fatty acid content of esterified lipids, samples must first be hydrolyzed to quantitatively cleave the sn-1 and sn-2 fatty acyl chains. We will use alkaline hydrolysis in which samples will be mixed with 0.3 M KOH in 80% methanol and incubated at 80°C for 30 min. After cooling to room temperature, formic acid will be added to stop the reaction followed by addition of hexane and mixed. After centrifuging, the top hexane layer is transferred to an LC vial and dried under a gentle stream of nitrogen. Reconstitution in methanol will produce an LC-ready sample. Our preliminary results (Figure inserted above with other figures), collected by an undergraduate, illustrate our ability to quantitatively hydrolyze a phospholipid test mixture.

Another important set of experiments performed related to Task 1 involve extraction of

phospholipids from V. cholerae grown with different concentrations of PUFAs, different exposure times to PUFAs, and in media differing in key abiotic factors (pH, salinity, temperature). These samples have been processed but still need analysis because the DHON student chose not to complete the thesis.

Regarding Aim 2: There was significant delay with regard to obtaining some of the antimicrobial peptides required to fully address Task 2. But in the end, the amount of data that will come from this funding will be staggering; we were able to perform MIC assays on 2 of 3 proposed AMPs (cecropin A and LL-37), but we were able to pivot to other AMPs and antibiotics (Novobiocin, melittin, erythromycin, and rifampin). We also confirmed the extraordinary lowering of MIC for colistin when PUFAs are available. This data in particular was featured on our R15 application that will be reviewed in October 2023.

Aim 3 consisted of computational modeling of the membrane consequences for substitution of fatty acids with and without simulation with antibiotics and AMPs. Advances were made regarding awareness of how many molecules of antibiotic to use for simulations; enough to show that it will be possible to create molecular dynamic simulations for predictive and comparative purposes.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Quantitation of PUFA incorporation	Proof of concept achieved; Application in process
MIC determination using PUFA and AMP combinations	Preliminary MICs determined for 10 AMPs and two cyclic peptides
Permeability assays using PUFAs and AMPs	Still in process, primarily due to scarcity of AMPs based on high cost of each peptide
Molecular Dynamics Simulations of antimicrobials using exogenous fatty acid-remodeled outer and inner membranes	Successful simulation achieved for polymyxin B and colistin; preliminary data obtained for 3 proposed AMPs; Data analysis still ongoing

Challenges & Strategies Used to Address / Overcome:

Task 1 proceeded relatively as expected; the main difficulty related to the difficult analysis necessary for interpreting the spectral data. Importantly, enough progress was made to include some data in the R15 application.

The main setback (for Task 2) was reagent availability during the first year due to Covid-19. The other challenge for Task 2 was the amount of peptide needed to perform both MIC and permeability assays; in many cases, we had to focus on MIC, which is certainly the most biomedically relevant data.

Task 3 made considerable progress while the graduate student was working the first year. A significant slowdown on that front occurred after the student graduated and we are still interpreting the large amount of data collected. The efforts by co-PI Harris and his graduate student significantly bolstered the 3rd aim of our recent NIH R15 application.

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

There were several surprises with regard to MIC results. The bacteria became more resistant to LL-37, melittin, and cecropin-A when given access to the PUFAs; the most significant was with 22:6 and cecropin A increasing the MIC 4-fold and 20:4 and 22:6 increasing MIC of melittin by 4-8 fold respectively. We were excited to see a significant decrease in MIC (4-fold) to erythromycin with 20:4 and 22:6.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The opportunity to pursue this line of research has shown us the potential for further funding. The PI hopes that accomplishments from this grant will impact his upcoming application for promotion to full professor. But more importantly the PI is primed for producing even more data related to the project that will enable external funding opportunities and continue to pave the way for successes in the area of research. Likewise, the project has benefited Dr. Harris during his tenure as an associate professor. Overall, the collaboration was strengthened and will be validated by acquisition of external funding. We are positioned to prepare additional applications to the NIH and NSF, equipped with preliminary data made possible through this grant. The PI will be on Professional Development Leave next semester, which is good timing for compiling data from this grant into external funding opportunities.

Students Impacted

Andrew Turgeson, Ph.D. student, Department of Chemical Engineering: first author on publication; generation of data for future manuscripts; excellent experience for his post-doc application.

Naina Patel, undergraduate student, Department of Biology, Geology and Env. Science: received support from the grant as she performed experiments for her departmental honors project. Naina will graduate in December and her data has been presented at a research conference and will be preliminary data in a grant application.

Benjamin House, undergraduate student, Department of Chemistry and Physics: Ben spearheaded the preparative TLC and UPLC/MS studies during the summer of 2022. He continues to be compensated from the grant and is working on analysis of data. Because of the CEACSE, Ben began working on another project in my laboratory and saw it to completion, earning authorship and padding his application for medical school (accepted to Vanderbilt).

Saksham Saksena, undergraduate student, Vanderbilt University: Saksham was my REU student during the summer of 2022. He was able to interact with students and myself working on the CEACSE, which undoubtedly benefitted from his perspective on his own bioinformatics project which was published during the funding period.

Lucas Morley, undergraduate student, University of Pittsburgh: Andrew Turgeson (and Dr. Harris) trained Lucas (an REU student) on how to generate molecular models of membranes and associated simulations. His training was enriched due to the CEACSE-related data and opportunities.

Olivia Chester, undergraduate student, UTC: Olivia gained training during the project and made contributions to the data on this grant as well as another collaborative project.

Meredith Grant, undergraduate student, UTC: Meredith was trained and has become an expert at performing MIC assay, many of which pertained to this project.

Mallory Anderson, undergraduate student, UTC: Mallory also gained experience and learned MIC assays that informed the project. She graduated May 2023 and was trying to gain employment in Germany.

Community and Broader Impacts

There are substantial broader impacts to this research, including basic scientific exploration of how bacterial membranes can adapt depending on available fatty acids in their environment. Not only does this have relevance for all organisms, but it reveals an unexplored field that could increase our understanding of cellular survival and adaptation in a variety of settings; of particular interest are those adjustments that impact pathogenesis and human infection. The PI and co-PIs will continue to investigate pathogens of both humans and animals to decipher the membrane dynamics underlying fatty acid-mediated membrane lipid homeostasis. The most intriguing angle currently is identifying PUFA and AMP combinations that lower the MIC and could be utilized in clinical setting as treatment options. The PI also plans to explore the impacts of this phenomena on aquaculture, as he will travel to the Virginia Institute of Marine Science (VIMS) in Spring 2024 to collaborate with researchers studying the deleterious effects of *Vibrio* species on oyster populations.

Scholarly Products

Publications:

Saksena S., K. Forbes, N. Rajan and D. Giles. 2023. Phylogenetic investigation of Gammaproteobacteria proteins involved in exogenous long-chain fatty acid acquisition and assimilation. *Biochem Biophys Rep* 35: 101504. https://doi.org/10.1016/j.bbrep.2023.101504.

Impact Factor: 2.7

Hofer R.N., A. Lin, B.J. House, C.N. Purvis, B.J. Harris, S.J.K. Symes and D.K. Giles. 2023. Exogenous polyunsaturated fatty acids (PUFAs) influence permeability, antimicrobial peptide resistance, biofilm formation, and membrane phospholipid structure in A-layer and non-A-layer strains of *Aeromonas salmonicida. J Fish Dis* 46(1):31-45. doi: 10.1111/jfd.13715. Epub 2022 Sep 11.

Above average research output (57th percentile) in Altmetric; Impact Factor: 2.5

Turgeson A., L. Morley, D. Giles and B. Harris. 2022. Simulated docking predicts putative channels for the transport of long-chain fatty acids in *Vibrio cholerae*. *Biomolecules* 12(9):1269. doi: 10.3390/biom12091269.

Impact Factor: 5.5

External Conferences:

1. Saksena, S. & Giles, D. Phylogenetic Investigation of Gammaproteobacteria Proteins involved in Exogenous Long-Chain Fatty Acid Acquisition and Assimilation. Vanderbilt Undergraduate Research Fair. Vanderbilt University, Nashville, TN. September 8, 2022.
2. Patel, N. & Giles, D. Polyunsaturated fatty acids affect membrane permeability and antimicrobial activity of polymyxin B and colistin on *Vibrio cholerae*. Association of Southeastern Biologists Annual Meeting. Poster presentation. Little Rock, AR. March 2022.
3. Chester, O. & Giles, D. The effects of polyunsaturated fatty acids in the presence of piscidins on Vibrio cholerae. Association of Southeastern Biologists Annual Meeting. Poster presentation. Little Rock, AR. March 2022.
4. Giles, D. MAGA! Make Antibiotics Great Again! Association of Southeastern Biologists Annual Meeting. Oral presentation—Lightning Talk. Winston-Salem, NC. March 2023.

Presentations at UTC:

- 1. Patel, N. & Giles, D. Polyunsaturated fatty acids affect membrane permeability and antimicrobial activity of polymyxin B and colistin on *Vibrio cholerae*. UTC Research Dialogues. Poster presentation. April 2022.
- 2. Morley, L., Turgeson, A. & Harris B. Comparing *Vibrio cholerae* FadL homologs by simulated docking and knot theory topological measurement. UTC iCompBio REU Final presentations. https://youtu.be/JdA8zGtqQbU
- 3. Saksena, S. & Giles, D. Phylogenetic Investigation of Gammaproteobateria Proteins involved in Exogenous Long-chain Fatty Acid Acquisition and Assimilation. UTC iCompBio REU Final presentations. https://youtu.be/XoikOiPCHw8
- 4. House, B. Quantifying the Uptake of Exogenous PUFAs in *Vibrio cholerae*. UTC Chemistry and Physics URP Oral Presentation. Summer 2022.
- 5. House B. C., Lin A., Giles D. K., Symes S. J. K (2022) Polyunsaturated fatty acid incorporation into membrane phospholipids of *Aeromonas salmonicida*. SERMACS, San Juan Puerto Rico, Oct 2022, Poster.

Inventions or Other Intellectual Property

Inquiries have been made regarding the potential for developing therapeutics based on this research; however, there is still a substantial amount of work to achieve commercialization. The PI leveraged this project into applying for a FLY Pitch Competition for Researchers (UTC), in which he won 2nd place and $10,000 to expand and complement this line of research. Furthermore, the preliminary data obtained in the CEACSE also bolstered the PIs application for a Harris Commercialization Grant (UTC College of Business) that was awarded in the amount of $6,000.

Research Outreach & Collaboration

Aside from continuing the current collaboration with Drs. Harris and Symes, the PI has been strengthening his collaboration with Dr. Myriam Cotten, an Applied Chemist at William and Mary. Together, they are exploring the impact of fish AMPs (piscidins) on Gram negative bacteria and how PUFAs may alter survivability in aquatic environments.

EXTERNAL FUNDING

Proposal Submissions

- NIH R15. *In vitro and in silico investigations of changes in bacterial cell membrane dynamics due to polyunsaturated fatty acid (PUFA) modifications. $396,750. Submitted June 2023.*

Contracts/Awards Received

- UTC FLY for Researchers 2nd Place Prize ($10,000)
- UTC Harris Commercialization Grant ($6,000)
- UTC Ruth S. Holmberg Grant for Faculty Excellence ($5,000)
- From Previous CEACSE award: Experimentally Guided Modeling and Simulation for Cholera Dynamics. (PI: J. Wang; Co-PIs: D. Giles, B. Harris) $300,000. 2019-2023

Sponsored Program Capacity Building Activities

- The PI did participate in a Summer Grant Writing workshop sponsored by the College of Arts and Sciences during summer 2021.

WHAT'S NEXT FOR THIS RESEARCH?

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

In the short term, I anxiously await Professional Development Leave, which will afford the opportunity to digest all of the data and decide on which grants would be most appropriate to apply. Also, we are still benefiting from the materials purchased and will add large amounts of data in the next year that could open further opportunities.

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

Essentially answered in the previous question, I expect to continue working with Drs. Harris and Symes to further this line of research. I am also actively pursuing new collaborative endeavors with Dr. Myriam Cotten at William and Mary and Dr. Kimberly Reece, Chair of Aquatic Health Sciences at VIMS**.**

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

There are two potential barriers for advancing this research: funding and translation from in vitro to in vivo. The funding will be actively pursued through external grant applications, while the PI continues to identify a collaborator that has an animal model that would establish the necessary translational validity to the overall hypothesis that PUFAs can alter antibiotic treatment regimens in ways that benefit the patient.

FINANCIAL ACCOUNTING

To my knowledge all available funds were spent; there were a few items that were not going to arrive until after the funding period, so we had to pivot to other materials.

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Hamdy Ibrahim, Lead PI

Co-PI(s): Eleni Panagiotou
Other Personnel: N/A

Project Title: "Topological design of porous metals for biomedical application"

Date Submitted: October 2019

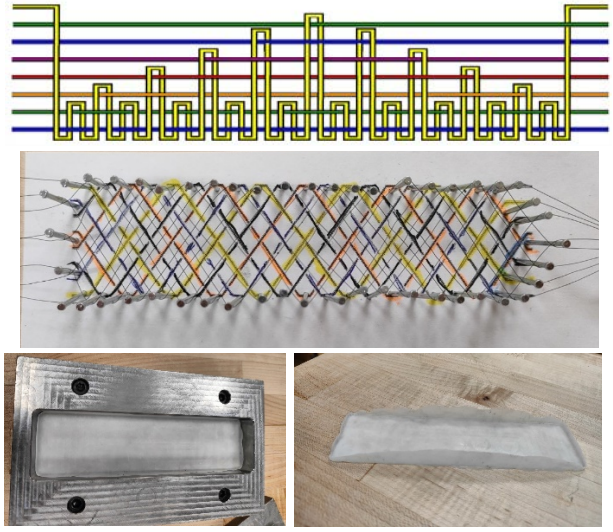
Award Start – End Date: July 1, 2020 – June 30, 2023

Non-Technical Summary:

This proposed research is focused on the creation of optimal biodegradable metal material for biomedical applications using tools from topology. In particular, we focus on the development of such materials for the use in bone implants. It has been shown that the distribution of pores in bones and their geometry plays a fundamental role in their ability to bear the load of the body. With this research we test the hypothesis that the overall topology of the porous structure, and not only the average size of porous or their distance, can provide more refined information to characterize different structures and to provide optimal structures. We will combine computer simulations and topological data analysis, and tools from braid theory and graph theoretical approaches. We will propose optimal structures of controlled topology that will be created in the laboratory with established modern techniques, such as 3d-printing, and with new methods, such as entangled metal wires. Our approach is expected to provide a new systematic way of studying biodegradable metal material for bone implant applications. This will lead to the application for external funding to study such material on a bigger scale in order to make an impact on medicine and industry.

PROJECT TITLE: “Degradation Topological design of porous metals for biomedical application”
Technology Area of Interest: Health & Biological Systems

TECHNICAL APPROACH	OUTCOMES
• Creation of new topologically optimal biodegradable porous configurations using one of two methods: continuous metal porous material and/or metal wire porous material. • Fabrication of the topological structures for biomedical application based on the investigated theories. • Testing the mechanical properties of the created topological structures.	• Configurations and designs based on the braid theory were developed. • Self and inter-entangled metal wires were fabricated, whose global topology mimics that of metal porous material. • The mechanical properties of the created metal wire-based structures were assessed and compared to the expected ones from the modeling theory.

RESULTS	OTHER INFO
	**Budget and Schedule** Total Budget: $92,955.00 Actual Used: $84,166.38 Balance: $ 8,788.62 Total period of performance is 24 months. Task 1: Months 1-6 Task 2: Months 6-9 Task 3: Months 9-18 Task 4: Months 18-24 **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

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Creation of new topologically optimal biodegradable porous configurations using one of two methods: continuous metal porous material and/or metal wire porous material.	New topological designs/configurations were developed.
Fabrication of the topological structures for biomedical application based on the investigated theories.	The proposed topological structures were fabricated using different fabrication methods.
Testing the mechanical properties of the created topological structures.	The mechanical properties were assessed and compared to those based on theory.

Challenges & Strategies Used to Address / Overcome:

The PIs struggled to conduct any of the research activities during the first year (2020/2021) due to the pandemic restrictions. This was followed by a great challenge to hire students (graduates in particular) in the first and second years of the project as a result of the Covid restrictions, especially on international students. Despite these difficulties, the team managed to hire some students (graduate and undergraduate) for some of the project semesters, especially in the last 2 years. Another challenge that the team faced was that the lead PI Dr Panagiotou accepted a position at another university and had to leave the UTC in the middle of the project period. That caused a lot of delays and difficulties in completing the project activities, which the team dealt with by having more virtual meetings and increasing the time commitment of the Co-PI to the project.

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

N/A

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The project helped the PIs to work together and submit a proposal to the University of Tennessee-Oak Ridge Innovation Institute (UT-ORII) Seed Funding program.

Students Impacted

- Hemanth Kumar, master's student: He worked on the project, and he was fully funded. He was a student in the Math Department at UTC.
- Rahul Kshatri, master's student: He worked on the project, and he was partially funded from the project for one semester. He was a student in the Mechanical Engineering Department at UTC.

- Vipul Patil, master's student: He worked on the project, and he was partially funded from the project for two semesters. He was a student in the Mechanical Engineering Department at UTC.
- Gage Plotner, Undergraduate student: He worked on the project, and he was partially funded for one semester.

Community and Broader Impacts

Metal porous material is used in biomedical applications and model biological materials, such as bones and bone implants. Another important aspect of the proposed project is that it consists of an interdisciplinary effort to bring together researchers from Mathematics, Mechanical Engineering and the SimCenter. In addition, this grant has educational objectives. Graduate and undergraduate students were supported directly by the grant, were trained and contributed to the projects, gaining both knowledge and experience in the research process. Moreover, the list of collaborators promotes the underrepresented group of women scientists in Mathematics.

Scholarly Products

Publications:

N/A

External Conferences:

- **Ibrahim, H.**, (2022, June), High-strength and corrosion-controlled magnesium-based bone implants, TechConnect World Conference and Expo, Washington DC.
- **Ibrahim, H.** (2022, October). Biodegradable Magnesium-based Bone Fixation; Alloy Design, Post-fabrication Processes, and Biocompatibility. **Invited talk** in the *Materials Science & Technology (MS&T)*. Pittsburgh, PA.

Presentations at UTC:

- Vipul Patil, Ron Balanay, Eleni Panagiotou & **Hamdy Ibrahim** (2023, April). Biodegradable Metallic Braided Structures for Biomedical Implant Applications. *UTC Research Dialogue*. Chattanooga, Tennessee.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

The project helped the PIs to work together and submit a proposal to the University of Tennessee-Oak Ridge Innovation Institute (UT-ORII) Seed Funding program.

EXTERNAL FUNDING

Proposal Submissions

- E. Panagiotou (UTC), J-M. Carrillo (ORNL), M. Doxastakis (UTK), J. Gounley (ORNL), H. Ibrahim (UTC) & R. Kumar (ORNL) “Topological Material”, submitted to the the University of Tennessee-Oak Ridge Innovation Institute (UT-ORII) Seed Funding program, 2021. Requested amount: $62,486. Status: Not Funding.

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?

The PIs will continue their work on the explored areas of research and will leverage the acquired tools and knowledge to follow-on studies and proposals.

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 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Hamdy Ibrahim, Lead PI

Co-PI(s): Mohammad Mahtabi
Other Personnel: N/A

Project Title: “Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants”

Date Submitted: October 2020

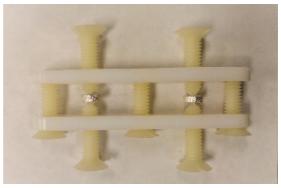
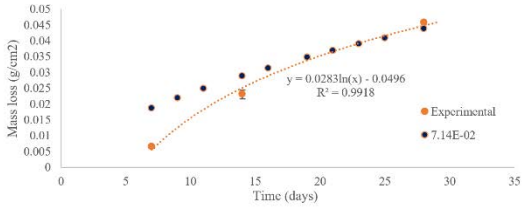
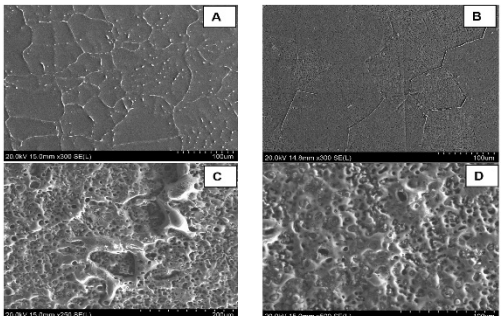
Award Start – End Date: July 1, 2021 – June 30, 2023

Non-Technical Summary:

Magnesium and its alloys have been under extensive research recently due to the high potential of their use for biomedical implant applications. For instance, the use of bone implants made of magnesium that can offer the required stability during the healing period and subsequently degrades is expected to result in a clinical breakthrough by eliminating the problems associated with the standard-of-care permanent implants such as stress shielding. Understanding the corrosion behavior of magnesium-based implants is crucial to assure the biomechanical performance of these new devices. In this project, we propose to develop a numerical model that can simulate the corrosion behavior of magnesium implants coated with biocompatible ceramic coatings. This model will serve as a future design tool for studying patient-specific biodegradable implants and support our project long-term goals.

PROJECT TITLE: "Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants"
Technology Area of Interest: Health & Biology Systems

TECHNICAL APPROACH	OUTCOMES
• Developing a numerical model based on the physical modeling approach to simulate the corrosion rate of coated Mg. • Designing and creating a ceramic-based coating on the surface of the Mg alloy using micro arc oxidation process. • Calibrating and validating the developed model via performing a series of in vitro corrosion tests for our coated Mg alloy samples in conditions simulating those in the physiological environment. • Using the validated code to simulate the in vitro corrosion rates of patient-specific implant devices (plates and screws).	The code was developed based on the physical modeling approach and the model was calibrated by conducting a series of tests in conditions simulating the body environment. This project resulted in 4 journal publications, 6 conference presentations, and 3 submitted external grant proposals.

RESULTS	OTHER INFO
   Figure 45 Numerical vs. experimental data for coated pure magnesium. 	**Budget and Schedule** Total Budget: $95,111.00 Actual Used: $93,924.18 Balance: $ 1,458.58 Total period of performance is 24 months. Task 1: Months 1-6 Task 2: Months 6-9 Task 3: Months 9-18 Task 4: Months 18-24 **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

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Developing a numerical model based on the physical modeling approach to simulate the corrosion rate of coated Mg.	The model was developed based on the physical modeling approach.
Designing and creating a ceramic-based coating on the surface of the Mg alloy using micro arc oxidation process.	The coating process was established and used with the model.
Calibrating and validating the developed model via performing a series of in vitro corrosion tests for our coated Mg alloy samples in conditions simulating the physiological environment.	The calibration and validation processes of the developed model were completed.
Using the validated code to simulate the in vitro corrosion rates of patient-specific implants (plates and screws) created by 3D printing and MAO coating process.	The model was used to design and simulate the degradation rates of a composite coating made by the MAO coating process and for patient-specific parts (3D printed parts). The tools and knowledge acquired in this step have proven to be helpful for the next steps in this project.

Challenges & Strategies Used to Address / Overcome:

The main challenge that the team faced was the availability of students (graduate in particular) to be trained and to assist in achieving the project objectives. This can be attributed mainly to the Covid situation during the first year of the project and the difficulty in hiring new students, especially international students. Despite these difficulties the team managed to achieve most of the project objectives and completed all the project objectives during the one-year extension.

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

We learned that the last objective, which is related to patient-specific implants is much more challenging and time consuming than we originally thought.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The PIs gained a fundamental understanding of corrosion modeling of coated magnesium materials as a new class of regenerative skeletal fixation devices using the physical modeling approach. The project also has enhanced the available infrastructure for the PIs to conduct

future research in the area of biomaterials. Finally, the support and results of this project helped the PIs to prepare and submit two pending proposals to the NSF and one proposal to the DoD.

Students Impacted

- Ahmed Korra, master's student: He was partially funded. He graduated in Summer 2023.
- Shelby Hash, undergraduate student: She was partially funded in this project during Fall 2021 and Spring 2022.
- Andre Flores, undergraduate student: He was partially funded in this project during Fall 2022 and Spring 2023.
- Adrianne Glover, undergraduate student: She was partially funded in this project during Spring 2023 and Summer 2023.
- Joshua Rich, undergraduate student: He was partially funded in this project during Spring 2023 and Summer 2023.

Community and Broader Impacts

The broader impacts of the conducted work on the advancement of a medical device made of biodegradable metals are substantial. Current modalities of treating patients with bone trauma rely on the use of permanent and stiff bone fixation devices (e.g., Ti-6Al-4V and 316L stainless) that carry substantial risks of inflammation, infection, subsequent bone fracture, and bone resorption. This usually requires physicians to perform a second implant removal surgery after bone healing which increases the suffering of patients and the total operation cost. The success in developing nonpermanent bone fixation devices that can address the problems associated with the currently-in-use permanent ones will result in a clinical breakthrough. One graduate student and four undergraduate students were involved in this project. They learned the about technical aspects of the project in addition to presenting the results of their work at conferences and in journal papers.

Scholarly Products

Publications:

- Abdalla, M. & **Ibrahim, H.** 2021. A Physical Approach to Simulate the Corrosion of Ceramic-Coated Magnesium Implants. *Applied Sciences*, 11(15), p.6724.
- Abdalla, M., Sims, A., Mehanny, S., Haghshenas, M., Gupta, M., & **Ibrahim, H.** (2022). In Vitro Electrochemical Corrosion Assessment of Magnesium Nanocomposites Reinforced with Samarium (III) Oxide and Silicon Dioxide Nanoparticles. Journal of Composites Science, 6(6), 154.
- Jia, M. S., Hash, S., Reynoso, W., Elsaadany, M., & **Ibrahim, H.** (2023). Characterization and Biocompatibility Assessment of Boron Nitride Magnesium Nanocomposites for Orthopedic Applications. Bioengineering, 10(7), 757.
- **Ibrahim, H.**, Billings, C., Abdalla, M., Korra, A., & Anderson, D. E. (2023). In Vivo Assessment of High-Strength and Corrosion-Controlled Magnesium-Based Bone Implants. Bioengineering, 10(7), 877.

External Conferences:

- **Ibrahim, H.**, (2022, June), High-strength and corrosion-controlled magnesium-based bone implants, TechConnect World Conference and Expo, Washington DC.

- **Ibrahim, H.**, (2022, May), Preclinical in vitro and in vivo assessment of high-strength and corrosion-controlled magnesium-based bone implants, International Conference on Metallurgical Coatings and Thin Films (ICMCTF), San Diego, CA.
- Abdalla, M., Sims, A., Haghshenas, M., Gupta, M., & **Ibrahim, H.** (2021, October). Corrosion assessment of rare earth elements and magnesium-based nanocomposites for bio-implant applications. *Materials Science & Technology*. Columbus, Ohio.
- **Ibrahim, H.** (2022, October). Biodegradable Magnesium-based Bone Fixation; Alloy Design, Post-fabrication Processes, and Biocompatibility. **Invited talk** in the *Materials Science & Technology (MS&T)*. Pittsburgh, PA.
- Hash, S., Jia, M., Diaz., W., Elsaadany, M., & **Ibrahim, H.** (2022, October). Magnesium-Based Nanocomposites for Bone Fracture Repair. *Materials Science & Technology (MS&T)*. Pittsburgh, PA.
- Billings, C., Abdalla, M., Anderson, D., & **Ibrahim H.** (2022, August). Preclinical biocompatibility assessment of high-strength and corrosion-controlled magnesium-based bone implants. In *14th Symposium on Biodegradable Metals for Biomedical Applications*, Alicante, Spain.

Presentations at UTC:

- Hash S., Diaz, W., & **Ibrahim, H.** (2022, April). Corrosion assessment of biodegradable magnesium-based nanocomposites. *UTC Research Dialogue*. Chattanooga, Tennessee.
- Andre Flores & **Ibrahim, H.** (2023, April). Fabrication and characterization of magnesium-based nanocomposites for bone implant applications. *UTC Research Dialogue*. Chattanooga, Tennessee.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

This research project resulted in the establishment of a strong interdisciplinary collaborative work between Dr. Ibrahim (PI; College of Engineering at the University of Tennessee at Chattanooga; UTC), Dr. Dhar (PI, College of Veterinary Medicine at the University of Tennessee at Knoxville; UTCVM), and Dr. Anderson (Co-Investigator; UTCVM). They all worked together to submit a partnering grant proposal to the DoD, which is currently pending.

EXTERNAL FUNDING

Proposal Submissions

- **Ibrahim, H.** "CAREER: CAREER: Hybrid Surface Coating Toward Corrosion-Controlled Magnesium-Based Implants", submitted to the National Science Foundation (NSF), 2023. Requested amount: $556,776. Status: Pending.

- **Ibrahim, H.**, Dhar, M. & Anderson, D. "Bioactive magnesium implants with controlled degradation and biocompatibility for orthopaedic applications", CDMRP-IIRA program, submitted to the Department of Defense (DOD), 2023. Total requested amount: $1,913,757, requested amount at UTC: $797,276. Status: Pending.

- **Ibrahim, H.** "ERI: Fabrication and Corrosion Modeling of Biodegradable Synthetic Heart Valves", submitted to the National Science Foundation (NSF), 2022. Requested amount: $197,175 Status: Not Funded.

- **Ibrahim, H.** “CAREER: Degradation control of coated magnesium toward patient-specific biomedical implants”, submitted to the National Science Foundation (NSF), 2022. Requested amount: $524,289. Status: Not Funded.
- **Ibrahim, H.**, Dhar, M. & Anderson, D. “Bioactive magnesium implants with controlled degradation and biocompatibility for orthopaedic applications”, CDMRP-IIRA program, submitted to the Department of Defense (DOD), 2022. Total requested amount: $1,913,757, requested amount at UTC: $759,264. Status: Not Funded.
- **Ibrahim, H.** “Dissolving and patient-specific Mg-based implants for broken bones”, submitted to the UTC Fly for Researchers 2022 Pitch Competition, 2022. Requested amount: $20,000. Status: **Awarded**.

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?

I will continue my research on the biodegradable metals for the intended biomedical applications with more focus on expanding the collaboration to follow-on studies looking at an in vitro cytotoxicity testing and in vivo animal studies.

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

I will work on strengthening the well-established interdisciplinary collaborative work between me, Dr. Dhar and Dr. Anderson from the College of Veterinary Medicine at the University of Tennessee at Knoxville; UTCVM) to use the developed knowledge and tools in this work in developing a next generation of bone implant devices.

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 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Daniel Loveless, Lead PI

Co-PI(s): Don Reising
Other Personnel: N/A

Project Title: “Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)”

Date Submitted:

Award Start – End Date: July 1, 2021 – June 30, 2023 [specify correct start and end dates]

Non-Technical Summary:

Physical authenticity verification of integrated circuits is an unresolved but critical issue for commercial (IoT) and Department of Defense (DoD) systems. Currently, there exists no acceptable way to guarantee that an electronic part is not counterfeit or has not been tampered with, so the concept of "trust" in a mission-critical part, or one that may contain sensitive personal data, is problematic. Most efforts to combat electronic counterfeiting have been focused on the digital layers. However, as wireless connectivity is becoming increasingly prevalent, there is a new opportunity to significantly enhance security through the RF, analog, and mixed-signal layers.

INFORM introduces a tamper forensic technique that provides post-fabrication imaging (termed ionizing radiation effects or IRES) of an integrated circuit (IC) through radiation and RF measurements. Coupled with machine learning, the technique pushes the boundaries of forensic analysis of the most advanced microelectronic fabrication technology nodes. The effort has resulted in four new publications, spurring interest in the DoD community; consequently, two new contracts (a Phase I STTR-complete and a basic research grant through the DTRA/Penn State University research consortium) were established to further develop the technique. Finally, the work has been presented to the international microelectronics radiation effects community on several occasions, leading to several new collaborations and plans for commercialization.

PROJECT TITLE: "Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)"

Technology Area of Interest: Advanced Modeling and Simulation; High Performance Computing

TECHNICAL APPROACH

INFORM introduces a tamper forensic technique that provides post-fabrication imaging of an integrated circuit (IC) through radiation and RF measurements. Specific tasks are:

- Conduct two-photon laser experimentation at NRL
- Design image processing techniques to visualize laser data
- Register "golden" cells to laser data (ChipSure)
- Develop and analyze dataset of IRE and URE waveforms for RF-DNA

OUTCOMES

(1) *T. Peyton, B. Dean, J. L. Carpenter, M. Fadul, D. R. Reising, and T. D. Loveless, "Supervised Learning and Classification of Single-Event Transient Anomalies,"IEEE Trans. Nucl. Sci., Apr. 2023.*

(2) *B. Dean, T. Peyton, J. L. Carpenter, D. Sam, A. Peterson, J. Kim, S. P. Lawrence, M. Fadul, D. R. Reising, and T. D. Loveless, "Machine Learning Approaches for Analysis of Total Ionizing Dose in Microelectronics," IEEE RADECS., Oct. 2022.*

(3) *J. L. Carpenter, B. Dean, S. P. Lawrence, R. D. Young, D. R. Reising, and T. D. Loveless, "Analysis of Single Event Transients in Arbitrary Waveforms Using Statistical Window Analysis," IEEE Trans. Nucl. Sci., vol. 70, no. 4, pp. 478-485, Feb. 2023. doi: 10.1109/TNS.2023.3243496.*

(4) *INVITED* "Hardening-By-Design Techniques for Analog and Mixed-Signal ASICs," by T. D. Loveless, presented at the 18th International School on the Effects of Radiation on Embedded Systems for Space Applications (SERESSA), CERN, Geneva, Switzerland, Dec. 2022.

(5) *INVITED* "Space Radiation Effects in Microelectronic Systems," by T. D. Loveless, presented at the Tennessee Technological University, Cookeville, TN, Sept. 2021.

(6) *INVITED* "Hardening Techniques for Analog and Mixed-Signal Circuits," by T. D. Loveless, presented at the 2021 IEEE Nuclear Space and Radiation Effects Short Course, Virtual, July 2021.

(7) "Supervised Learning and Classification of Single-Event Transient Anomalies," by T. Peyton, B. Dean, J. L. Carpenter, M. Fadul, D. R. Reising, and T. D. Loveless (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.

(8) "Functional Redundancy for Mitigation of SEE in Heterogeneous Computing Systems," by S. Camp, J. Carpenter, T. Skjellum, D. Reising, and T. D. Loveless (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.

(9) "Detection of Single Event Transients in Arbitrary Waveforms Using Statistical Window Analysis," by J. L. Carpenter and T. D. Loveless (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.

(10) "Towards AI-Based Mitigation of SEE," by T. D. Loveless, J. Carpenter, B. Dean, S. Lawrence, R. Young, and D. Reising (2021). 2021 Single Event Effects Symposium. La Jolla, CA (Virtual).

New grants:

- Missile Defense Agency (MDA) Phase I STTR Sub-contract to CFD Research Corporation, (12/21 – 8/22), Budget: $45,935
- Defense Threat Reduction Agency (DTRA) IIRM Consortium Member (9/22-12/23), Budget: $185,000

RESULTS

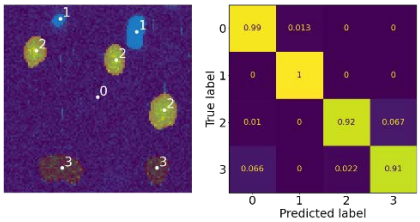


Figure 1. Spatial mapping (left) of an integrated phase-locked loop circuit with internal nodes identified through IRES imaging. Greater than 90% accuracy in identification of nodes via a deep neural network.

OTHER INFO

Budget and Schedule

Total Budget:	$90,000.00
Actual Used:	$88,579.79
Balance:	$ 1,420.21

Total period of performance is 24 months.

Task 1: Months 1-12 , Task 2: Months 1-6

Task 3: Months 6-12+, Task 4: Months 8-12+

Deliverables

- Transient analysis tool to be published at nanoHUB.org
- Annual report detailing results, financials, and work plan to complete the project
- Publication(s)
- External and internal conference presentation

Organization Information

Electrical Engineering Department, CECS, UTC

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Physical authenticity verification of integrated circuits (ICs) is a critical issue for commercial (IoT) and Department of Defense (DoD) systems. Currently, there is no acceptable way to guarantee that an electronic part is not counterfeit or has not been tampered with, so “trust” in a mission-critical part or one that contains sensitive personal data may be problematic. Most efforts to combat electronic counterfeiting have been focused on the digital layers. However, as wireless connectivity becomes prevalent, there is a new opportunity to enhance security through the Radio Frequency (RF), analog, and mixed-signal layers. This proposed program tackled these challenging security problems resulting from the increased use of untrusted electronics through coupled fundamental theory, physical verification, RF measurement, and trust management.

Our approach, Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM), addressed security vulnerabilities originating in fabrication, packaging, and validation through the novel use of non-destructive optical imaging, RF measurement, and machine learning (ML). As a result, trusted microelectronics can be verified and maintained through multiple phases of design, fabrication, packaging, and validation. The project had two integrated objectives:

Objective 1 (ChipSure Image Registration and Trust Identity): A focused ionizing radiation source was used to excite electron-hole pair generation (i.e., to “inject” charge) in localized regions of an IC substrate to image the front-end-of-line (FEOL) in IC fabrication. The resulting device fingerprints were used to establish baseline identity.

Objective 2 (RF-DNA and ML Trust Management): RF measurement was used to extract unique features from device output and side-channel waveforms. These waveforms were analyzed using the Ionizing Radiation Effects Spectroscopy (IRES) code developed in the RES lab and were coupled to ChipSure using ML to determine the most important physical and electrical features for device discrimination.

A feedback loop between novel experimental characterization and ML trust resulted in (1) a non-destructive post-fabrication FEOL imaging technique, (2) new insights into the origins of RF features, and (3) the development of a forensic anti-tampering technique (ChipSure). The findings are used to address security vulnerabilities at the physical device level and the RF waveform level and propagate through the digital system level. Specific applications in the trusted U.S. supply chain are significant. Innovations include:

1. Anti-Tamper Forensics: Short of a captive supply chain, any microelectronic part must leave the developer’s direct control and scrutiny at some point during the acquisition cycle. During that time, an adversary could introduce additional circuitry or modify existing circuitry for nefarious purposes. Such modifications, adequately implemented and concealed, are undetectable to physical, functional, or electrical screening, yet, once activated, the potential breach of security is substantial. We have discovered a novel and unique method of screening parts for tamper using focused ionizing radiation as a non-destructive diagnostic tool. ChipSure provides a fingerprint of an integrated circuit uniquely tied to the physical

layout; this device fingerprint, when compared to a known chip mask extracted from initial design documents, can identify suspicious physical features. Any tamper of the physical layout, even if functionally dormant and electrically inactive, can be detected. We expect this method, once fully developed, to be useful both as a screening go/no-go test for part acceptance and as a diagnostic test to identify tamper locations within the IC for investigation and remediation.

2. Maintenance of Trust through RF Measurement: A second, enabling contribution to the integrated architecture includes advances in Specific Emitter Identification (SEI) through IRES analysis of output and side-channel waveforms. We have developed a methodology for performing identification of IC features through RF features and ML. The technique is applicable to any transient anomaly application.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Conduct two-photon laser experimentation at NRL	New relationship with NRL with access to state-of-the-art two-photon absorption laser. Multiple new experiments planned for FY23.
Design image processing techniques to visualize laser data	The IRES image analysis has been migrated to the Python programming language and is accessible via GitHUB. The tool has prompted a new contract via the DTRA IIRM program. We are also in the process of building an accessible version for the community via nanHUB
Register "golden" cells to laser data (ChipSure)	Successful image registration has been completed. Further, IRES coupled with deep learning was able to identify previously unknown features within the IC under study.
Develop and analyze dataset of waveforms for RF-DNA	Our techniques have been developed for analysis of systems in a software defined radio (SDR). Limited new data is available thus far but will be planned in FY23.

Challenges & Strategies Used to Address / Overcome:

Radiation experimentation is challenging and often requires extensive parts preparation and additional design and test kit development. Our experiments with the SDR required special preparation before conducting radiation effects that included de-capsulating the manufactured packaging. De-capsulating the hermetically sealed package typically involves chemical etching to ensure removal of the external materials without impacting the internal Si-based materials and wire or ball bonding. We contracted a company to help us with this process, which has been increasingly difficult for complex systems on chip. Every part we have attempted thus far has been damaged and has delayed our ability to conduct further experimentation. We will

continue to investigate methods for accomplishing this or attempt to access a radiation facility with higher energy capabilities, which would allow us to penetrate the packing materials.

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

N/A (see above for challenges)

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

Research outcomes from the INFORM program have enabled many invited talks and new collaborative proposals. The PI is an internationally recognized expert in radiation effects, and the RES Lab at UTC is now known by the community as experts in radiation analysis, especially with novel AI-based tools. The Co-PI has developed new experience in microelectronic radiation effects, and through collaboration with the PI, have led efforts to move forward new systems approached in the field. These new initiatives are improving the reputations of the PI and Co-PI and setting the stage for a new center of excellence at UTC.

Students Impacted

Jake Carpenter (GA), Berkay Dean (UG), Trevor Peyton (UG)

Community and Broader Impacts

Scholarly Products

Refereed Journals

1. T. Peyton, B. Dean, J. L. Carpenter, M. Fadul, D. R. Reising, and T. D. Loveless, "Supervised Learning and Classification of Single-Event Transient Anomalies,"IEEE Trans. Nucl. Sci., Apr. 2023.
2. B. Dean, T. Peyton, J. L. Carpenter, D. Sam, A. Peterson, J. Kim, S. P. Lawrence, M. Fadul, D. R. Reising, and T. D. Loveless, "Machine Learning Approaches for Analysis of Total Ionizing Dose in Microelectronics," IEEE RADECS., Oct. 2022.
3. J. L. Carpenter, B. Dean, S. P. Lawrence, R. D. Young, D. R. Reising, and T. D. Loveless, "Analysis of Single Event Transients in Arbitrary Waveforms Using Statistical Window Analysis," IEEE Trans. Nucl. Sci., vol. 70, no. 4, pp. 478-485, Feb. 2023. doi: 10.1109/TNS.2023.3243496.

Invited Presentations

1. INVITED "Hardening-By-Design Techniques for Analog and Mixed-Signal ASICs," by T. D. Loveless, presented at the 18th International School on the Effects of Radiation on Embedded Systems for Space Applications (SERESSA), CERN, Geneva, Switzerland, Dec. 2022.
2. INVITED "Space Radiation Effects in Microelectronic Systems," by T. D. Loveless, presented at the Tennessee Technological University, Cookeville, TN, Sept. 2021.
3. INVITED "Hardening Techniques for Analog and Mixed-Signal Circuits," by T. D. Loveless, presented at the 2021 IEEE Nuclear Space and Radiation Effects Short Course, Virtual, July 2021.

Conference Presentations

4. “Supervised Learning and Classification of Single-Event Transient Anomalies,” by T. Peyton, B. Dean, J. L. Carpenter, M. Fadul, D. R. Reising, and T. D. Loveless (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.
5. “Functional Redundancy for Mitigation of SEE in Heterogeneous Computing Systems,” by S. Camp, J. Carpenter, T. Skjellum, D. Reising, and T. D. Loveless (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.
6. “Detection of Single Event Transients in Arbitrary Waveforms Using Statistical Window Analysis,” by J. L. Carpenter and T. D. Loveless (2022). 2022 Single Event Effects Symposium. La Jolla, CA, May 2022.
7. “Towards AI-Based Mitigation of SEE,” by T. D. Loveless, J. Carpenter, B. Dean, S. Lawrence, R. Young, and D. Reising (2021). 2021 Single Event Effects Symposium. La Jolla, CA (Virtual).

Inventions or Other Intellectual Property

We are currently in the process of obtaining an open-source license for our IRES code. The possibility of using tools developed using the code, however, will be discussed for potential commercialization opportunities.

Research Outreach & Collaboration

New collaborations have been started with Dr. Adrian Ildefonso at the Naval Research Laboratory. We are starting b-weekly collaboration calls in Sept. 2022 and will be using the facility for laser experimentation yearly.

New collaboration with CFD Corporation (Dr. Karthik Linga and others) has already resulted in one awarded Phase I STTR. We are currently in the process of writing two new proposals (in collaboration with the Critical Infrastructure Thrust Area).

EXTERNAL FUNDING

Proposal Submissions

1. Missile Defense Agency (MDA) Phase I STTR Sub-contract to CFD Research Corporation, (12/21 – 8/22), Budget: $45,935 (awarded)
2. Missile Defense Agency (MDA) Phase II STTR Sub-contract to CFD Research Corporation, (8/23 – 7/25), Budget: $650,000 (awarded)
3. Defense Threat Reduction Agency (DTRA) IIRM Consortium Member (9/22-12/23), Budget: $185,000 (awarded)

Contracts/Awards Received

1. Missile Defense Agency (MDA) Phase I STTR Sub-contract to CFD Research Corporation, (12/21 – 8/22), Budget: $45,935 (awarded)
2. Missile Defense Agency (MDA) Phase II STTR Sub-contract to CFD Research Corporation, (8/23 – 7/25), Budget: $650,000 (awarded)
3. Defense Threat Reduction Agency (DTRA) IIRM Consortium Member (9/22-12/23), Budget: $185,000 (awarded)

Sponsored Program Capacity Building Activities

- Partnership with SCALE microelectronics workforce dev program (~$400k funding)
- Technical chair of NASA NEPP SEE/MAPLD Workshop, La Jolla, CA, 2022
- Local Arrangements chair of the IEEE NSREC, Provo, Utah, 2022
- Participant in (1) TAMU Heavy-Ion Training Workshop, (2) NASA NSRL Training Workshop, (3) MSU FRIB Heavy-Ion Testing for DoD, (4) NASA ETW

PLAN FOR COMPLETION DURING THE NEXT FISCAL YEAR (EXTENSION PERIOD)

N/A

WHAT'S NEXT FOR THIS RESEARCH? [FILL IN AS APPROPRIATE FOR ANNUAL REPORTS, WILL BE REPEATED IN YOUR FINAL REPORT]

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

Develop IRES through the DTRA IIRM funding. This will likely lead to 2-year option funding in CY2024-2025. We hope to have a solid commercialization plan in place during this time, documenting our successes with the open-source IRES code.

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

Substantial growth (opportunity) is expected in microelectronics and more specifically in radiation effects. The relationships developed under the CEACSE program will be leveraged to lead many of these new efforts, including in advanced semiconductors, integrated circuits, radiation effects, photonic integrated circuits, cryogenic systems, and quantum devices.

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?

Lack of critical mass and administrative support. The RES lab, and the work conducted within the Extreme Environments Thrust area is self-sustaining; however, further growth is not possible without a critical investment to aid in procurement of post-docs and new faculty in the area of microelectronics and radiation effects.

FINANCIAL ACCOUNTING

$1,420.21 of funds remain (1.5%). This is due to overestimation of fringe rates.

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Dr. Mohammad J. Mahtabi, Lead PI

Co-PI(s): Dr. Hamdy Ibrahim
Other Personnel: Mr. Saeed Ataollahi-Graduate Student (Research Assistant), Mr. Mitchell Bauer- Undergraduate Student (Research Assistant), Mr. Stephan Rodemann- Graduate Student (Research Assistant)

Project Title: “Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials”

Date Submitted: 09/20/2022

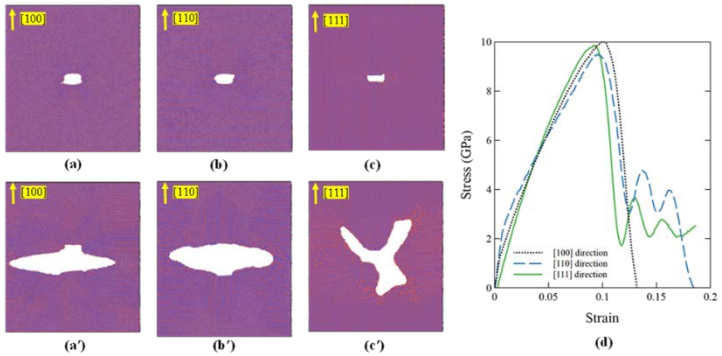
Award Start – End Date: July 1, 2021 – June 30, 2022

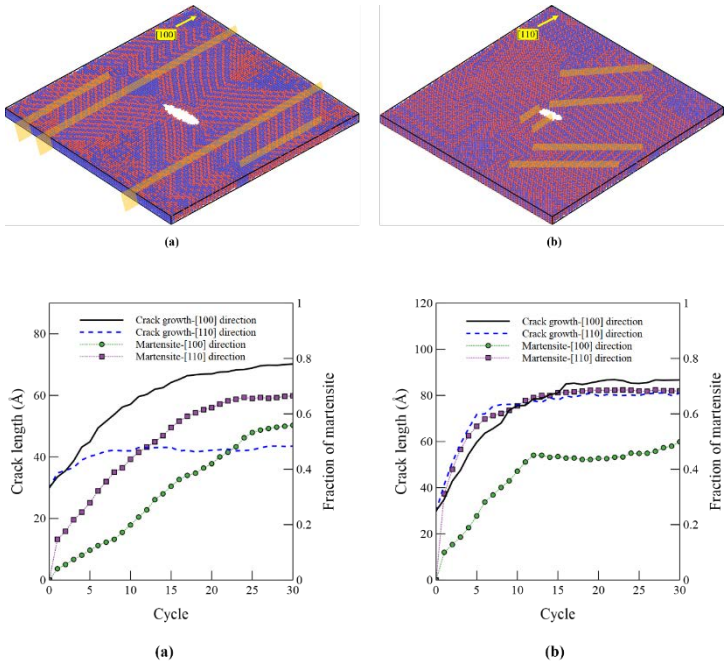
Non-Technical Summary:

Profound knowledge of materials is a key aspect of most industries such as automotive, aerospace, and biomedical. There is currently a race between various academic and industrial sectors to make more functional, stronger, and durable engineered structures, while keeping them lighter, more functional and more sustainable. In this regard, the manipulation of materials, their properties and the associated processes is key. In addition, materials science by nature is an interdisciplinary area which bridges various areas of engineering such as mechanical, chemical, biomedical and civil engineering. The Materials Genome Initiative (MGI) that was announced by the Obama administration in 2011 — to coordinate work across agencies such as the Department of Energy, NASA and others — indicates the significance of this area to the nation’s strategic plans.

With the rapid growth in computing power, multiscale simulations are now becoming a viable approach to calculate the properties of materials and design new materials. In this project, we developed interatomic potentials that describe atomic level interactions to computational model the response of advanced alloys made of nickel, titanium, and hafnium to various mechanical and thermal loads. The work results in models that play a major role in atomistic simulation of materials and can be used to engineer new materials for tailored properties. During this project, one PhD, one MS, and multiple undergraduate students were involved in research activities. As a result of this work one conference paper has been accepted for publication in an international conference, two abstracts were accepted for presentation in an international conference, and a manuscript is prepared to be submitted to a peer-reviewed journal. In addition, the results of this work enable the PIs to generate preliminary data that will be used to prepare external proposals. All these impacts are aligned with the missions of SimCenter.

PROJECT TITLE: "Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials"
Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
The calibration and validation of the interatomic potentials for HTSMAs starts with an initial guess of the MEAM potential, as well as experimental and first principal data, obtained by the Density Functional Theory (DFT) simulations. Once we have all the necessary data, the calibration of the initial potential to the data will be performed, considering that the calibration is targeted to obtain mechanical response of the material. List of tasks: Task 1. Literature review, DFT simulations, Task 2. Model calibration Task 3. Validation, MD simulations, preparing manuscripts	The outcomes of this project include one conference paper and presentation, three conference presentations, three journal papers, in addition to preliminary data and results for future journal papers as well as proposals to be submitted to external opportunities. The outcomes of this project also support the missions of UTC's SimCenter for establishing and expanding multidisciplinary computational work through mentoring students by involving multiple graduate and undergraduate students in the related research activities.
RESULTS	**OTHER INFO**
Developed interatomic potentials based on the Modified Embedded Atom Method (MEAM) for unary Ni, Ti, and Hf and their binary combinations. Also, conducted molecular dynamic simulations on the properties of binary NiTi to predict the beahvior of a nano-size crack inside the material.  	**Budget and Schedule** Total Budget: $90,000.00 Actual used: $89,574.17 Balance: $425.83 The total period of performance is 12 months. Task 1: Months 1-7 Task 2: Months 6-10 Task 3: Months 9-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Annual report detailing results, financials, and work plan to complete the project.



- Journal publications as well as external and internal conference presentation

Organization Information

Department of Mechanical Engineering, The University of Tennessee at Chattanooga, Chattanooga, TN, United States

E-mail: Mohammad-Mahtabi@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

In recent years, high temperature SMAs (HTSMAs) have been introduced that operate at temperatures well above 100 °C and offer high work output, which particularly suits them for applications in aircraft and car engines, and energy-generation systems. Until now, different types of HTSMAs, such as ternary alloys based on NiTi, CuAl, and CuZn have been developed for various applications. Among HTSMAs, ternary NiTi-X alloys (where X = Hf, Zr, Pt, Pd, or Au) have proved to offer enhanced mechanical and functional properties. Hf (and Zr) as the ternary element is of more interest than other elements due to the relatively lower cost and lower weight and a high slip resistance (>1 GPa). Furthermore, theoretical studies show a superiority of the transformation strains of NiTiHf (HTSMA of choice in the current work) compared to NiTi; transformation strains of up to 7% and 15% can be achieved in compression and tension, respectively, for NiTiHf. The chemical concentration of ternary addition is proven to play an important role on the final transformation temperatures (TTs) and mechanical properties of the alloy. For example, at chemical concentrations higher than 10% atomic of Hf, the TTs of NiTiHf alloy tend to increase linearly up to 525 ℃ for 30% atomic of Hf, when Hf is substituted for Ti. Thus, new applications can be developed for such HTSMAs. In general, more research is needed to improve the associated low workability and ductility resulting from the high hardness of Hf alloys. Workability and ductility are especially important when one considers the possibility of manufacturing HTSMAs into suitable sizes and shapes and for microstructure control. In addition, the advancement of the additive manufacturing (AM) technologies obliterates the challenges of formability of NiTi-based HTSAMs, thus making them more promising candidates for novel applications. Therefore, more accurate, less expensive ways, such as MD simulation, of

understanding the effect of various factors, will be a great enabler toward tailoring and improving the properties of these alloys and extending applications.

Despite the advantages and unique properties of NiTi-based HTSMAs, there are many aspects of these alloys that are unknown and there is much to be understood about the micromechanics and the mechanisms involved in the interplay of various factors affecting the thermomechanical properties of these alloys. Molecular Dynamics (MD) simulation provides a great tool to study such behaviors —especially at the atomic and molecular level— and understand the various factors affecting the properties of these alloys. In addition, due to the increasing trend toward structure miniaturization, MD simulations have become noticeably important, in the projection of new potential fabrication methods into reality.

With the rapid growth in computing power, multiscale simulations are now becoming a viable approach to calculate the properties of materials and design new materials. In this regard, ab initio simulations using Density Functional Theory (DFT), while ideal, are very limited in the size of the model due to computational costs. Molecular dynamics (MD) simulations present a promising alternative to DFT to computationally study the properties of materials. These methods are powerful because deformation properties of materials such as crack initiation and growth, dislocation behavior, polycrystal effects, effects of second phases, interface interactions, and so on, are naturally captured in these simulations. On the other hand, the accuracy of MD simulations heavily relies on the quality of the interatomic potentials. In this proposal, we propose the development of interatomic potentials, based on multi-objective optimization of parameters to present the mechanical properties of high temperature actuator materials (i.e., high temperature shape memory alloys, HTSMAs). The proposed research involves developing, calibrating, and validating interatomic potentials for MD simulations of alloys made of Ni, Ti, and Hf.

List of Objectives / Aims / Major Milestones Proposed	**Cumulative Outcomes / Accomplishments**
Literature review, DFT simulations	- DFT simulations have been completed for the pure Ni, Ti, and Hf. - Surface energies have been calculated based on DFT calculations for various crystal structures of the unary elements.
Model calibration	- Calibration of the MEAM potential constants have been done for unary interactions: i.e., Ti-Ti, Ni-Ni, and Hf-Hf interactions. - Additional codes have been developed to calculate the energy terms based on the DFT results. - Calibration of the MEAM potential constants have been done for binary interactions: i.e., Ni-Ti, Ni-Hf, and Ti-Hf interactions.

Validation, MD simulations, preparing manuscripts	- Validation with experiments and verification with other numerical methods have been done for binary and unary models. - MD simulations have been conducted on binary alloys of NiTi and resulted in one journal manuscript, one conference paper, and two abstracts accepted for conference presentations

Challenges & Strategies Used to Address / Overcome:

The development of interatomic potentials is, in general, very challenging due to the large number of involved parameters as well as the dependency of the results to different variables. We had to develop computer codes to run numerous DFT simulations. In addition, the appropriate method of calibrating the model parameters based on the large number of input variables was also challenging. We overcome these challenges by prioritizing the materials' response of interest.

Another challenge was the calibration of binary MEAM potentials that are the precursors to the final ternary interatomic potential. For instance, there is no experimental data for Ti-Hf, to be used for MEAM potential calibration. Enthalpy of formation, the equilibrium nearest-neighbor distance and the reference structure had to be modeled using DFT from scratch with trial-and-error approach to obtain the desired elastic constants. Furthermore, the large number of screening parameters in the ternary MEAM potential, which have a significant role in prediction of material properties, asked for numerous molecular dynamic simulations. This was done by automating the process of analyses (with consideration of reducing the model size effect). Days of simulations were performed using different bash scripts that changed the calibration parameters, ran the models and post-processed the results to narrow down the range of MEAM parameters for more detailed analyses.

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

In general, atomistic simulations based on DFT and MD methods are very powerful. However, appropriate modeling of some of the mechanical properties may be quite challenging using these methods, which can be due to several reasons. First, the limitedness of the time- and length-scale may prohibit obtaining desired results with limited number of (most of the time time-consuming) simulations. Furthermore, unlike the possibility of developing a systematic approach for calibrating binary MEAM potentials, doing so for ternary, and quaternary alloys is not straightforward and requires many trial-and-error to tune the parameters. This becomes even harder for special classes of materials, such as SMAs, where solid-state phase transformations are also expected in the thermomechanical response of the material.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI:

Since one of the long-term plans of our research team at UTC is to establish a strong computational program for materials science and engineering, and computational design of materials, this project assisted to build the foundation to reach some of our objectives. The project provided financial support for a PhD student (as graduate research assistant) and an undergraduate student (research assistant). This also enabled us to expand our current area of research and help the visibility of our research group through journal and conference publications/presentations. In addition, the partial summer salary greatly helped in dedicating the time on research activities and supervising students in their research. Furthermore, the support for this research resulted in preliminary data and tool development that have been used and will be used for submission of external proposals and expanding our research on computational materials science. This will greatly help the PI towards his tenure and promotion, where research and scholarly activities are requirements for it.

Impact on the Career of the Co-PI:

This project provided the opportunity for Dr. Ibrahim to expand his research area more into computational materials analysis. In addition, the partial summer salary in summer 2022 and provided him with the necessary time to dedicate to this research and increased his capacity to advance his career in this area.

Impact on the Career(s) of the Key Collaborators

- Saeed Ataollahi (PhD student, conducted the computational work and calibrating the potentials - expected graduation Dec. 2023) worked on this research. The results of this work will form a large portion of his PhD dissertation. So far in this project, he has co-authored two conference papers, two journal articles, and will be submitting two more journal articles.
- Mitchell Bauer (UG student): involved in research activities. Learned about science of materials, shape memory alloys (SMAs), and their processing. He has become very interested in research on materials and is seriously considering post-graduate studies.
- Stephan Rodemann: partially involved in the project to build a test-stage for testing SMAs for their thermomechanical properties. Mr. Rodemann attempte to build this device for this project and to conduct his research in a closely related area.

Community and Broader Impacts

Scholarly Products

Publications:

1. Ataollahi, S. and Mahtabi M.J., "Atomistic Simulation of Fatigue Crack Growth in Superelastic NiTi" is under preparation to be submitted to "Computational Materials Science" journal.

External Conferences:

- Ataollahi, S. and Mahtabi, M.J., 2022. "A Study on Fatigue Crack Growth in Single-Crystal NiTi Using Molecular Dynamics" IMECE22- International Mechanical Engineering Congress & Exposition- Virtual Conference: October 30 – November 3, 2022.
- Ataollahi, S., Mahtabi, M.J., 2022, “Atomistic Simulation of the nano crack growth in superelastic nickel-titanium alloys, ASTM international E08 committee meeting, November 2nd, New Orleans, USA.

Research Outreach & Collaboration

EXTERNAL FUNDING

Proposal Submissions

4. Mahtabi, M.J. (PI), "Actuation Fatigue and Crack Growth Behavior of Shape Memory Alloys", a collaborative proposal was submitted in October 2022 to NSF’s “Metals and Metallic Nanostructures” program, ~$500,000.
5. Mahtabi, M.J. (co-PI), Yang, S. (PI), 2023, “MRI: Acquisition of an Advanced Scanning Transmission Electron Microscopy for Multidisciplinary Research Activities”, NSF - National Science Foundation, $999,908

Contracts/Awards Received

Sponsored Program Capacity Building Activities

PLAN FOR COMPLETION DURING THE NEXT FISCAL YEAR (EXTENSION PERIOD)

WHAT’S NEXT FOR THIS RESEARCH?

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

The work of this CEACSE grant will be followed up by the following activities:

Next 1-2 year(s):

- Submit one more proposal to external funding agencies.
- Publish one or two additional journal articles based on the obtained results – next one year.
- Present our results in international and national conferences as well as UTC research dialogue.

Next 2-5 years:

- Extend the work to various aspects of it such as development of new ternary MEAM potentials (for other alloying elements) as well as designing new alloys by the computational capability that the results of this work provide.

- Submit proposals on computational design of new materials to national funding agencies such as NSF and DOE.

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

- Computational design of materials for extreme conditions such as high temperature applications, or biomedical applications with UTC (Dr. Ibrahim and Dr. Barisik) and external collaborators (Dr. Elahinia, University of Toledo).
- Designing nanostructured materials based on atomistic simulations for high fatigue resistance (Dr. Yadollahi, Purdue University NorthWest)

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

It would have been great (if such proposals continued) to be able to allocate budget to acquire research equipment supporting the needs of the proposal.

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

One of the main barriers towards achieving the goals of my research is the limited access to experimental facilities and Space. Since my research area requires the validation of the computational work with experiments, access to such equipment is critical to advance my research work. Currently, I have managed to mitigate this need by collaborating with other universities or finding the required data in the open literature. However, this may have its own challenges and having some essential equipment at UTC could be a major enabler for my future research.

FINANCIAL ACCOUNTING

The total approved budget of the project was $90,000.00. By June 30, 2022, the actual amount of fund spent was $89,574.17 was spent to support students', travel, PIs' summer salaries, and materials and supplies.

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Ashley Manning-Berg, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: “Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record”

Date Submitted: August 31, 2023

Award Start – End Date: July 1, 2021 – June 30, 2023

Non-Technical Summary:

Ancient organisms preserved in chert rocks can provide information about the environments in which they lived and are therefore crucial for our understanding of the environmental conditions on early Earth. Early life on Earth consists entirely of microorganisms that lived in a community of other organisms called microbial mats. Interactions between microbial communities and their requirements for life cause a mat to form colorful layers, where one community uses the metabolic byproducts of another community to thrive. Within these mats, heterotrophs, or organisms that feed off of other organisms, are active and decompose the individual microbes in the mats. This decomposition is often viewed as a loss of information; however, recently, it’s been documented that investigating what is lost during decomposition is another source of environmental information and provides a timeline for preservation.

The goal of this project was to build upon a previously published model with information gained from decomposition in a laboratory setting. Some of the data from a previous laboratory study was published in Geobiology and was able to describe the changes observed in individual microbes within a preserved microbial mat. This project extended the model in that paper by using microbial communities (mixtures) and lab-grown microbial mats. Final data collection is being done on the lab portion of the project and will result in a publication with an undergraduate student author. The previously published computer model was obtained from the authors of the paper and a MS student from Math spent a summer deconstructing the model in the software program R. Ultimately, we were unable to determine a way to incorporate morphological changes into the model. There is interest in the geobiology community to accomplish this goal, however, I am still looking for a computational biologist who can help change the code in the model. Hopefully, I have found someone to work with through networking in the summer of 2023.

PROJECT TITLE: “Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record”
Technology Area of Interest: Health & Biology Systems

TECHNICAL APPROACH	OUTCOMES
The goal is to reconstruct the previous model to incorporate data on taphonomic changes in biomass to correlate the TIP value (Manning-Berg et al., 2022) to microbial mat decomposition. At the same time, we will perform decomposition experiments to determine if the rate or pattern of decomposition changes in a microbial mat or in communities of microbes from that of bacterial and algal monocultures. Task 1: Explore the parameters in the previously published model and identify those that might be useful for modeling decomposition. Simultaneously set up the actualistic experiment. Task 2: Perform the actualistic experiment to see if microbial mats will behave similarly to monocultures of bacteria and algae. Document decomposition over the span of at least 15 weeks. Task 3: Apply the decomposition patterns and models to obtain TIP values and use the models to describe/define mats and consortiums like the monocultures from Manning-Berg et al., 2022 Task 4: Identify where the decomposition data fit into the parameters in the model that can be used to mimic the decomposition observed in lab. Find a way to quantify TIP values in the model.	The previous microbial mat model was reconstructed, works, and the code has been broken into annotated groups or chunks to get a better sense of which parameters affect specific outputs of the microbial mat. This includes the type of mat (modern vs. Precambrian) we are trying to model. Decomposition experiments have been more successful and have led to a presentation at the Southeast Geological Society of America conference in April 2022 and a poster presentation at the national Geological Society of America conference in October of 2022. The research has expanded to living microbial mats collected by new colleagues and has also sparked interest in understanding how one class of microorganisms decomposes because the literature points to the presence of these microbes in early Earth ecosystems; however, there is much debate on whether the descriptions are accurately labeled as this class of microbe. This research will likely lead to a publication by the end of the academic year.

RESULTS	OTHER INFO
From the model, we have been able to get a biomass concentration every 12 hours for 3 days after the spin-up of the model. It was unclear, however, how this number was obtained in the model and using the produced number did not yield results that were different from those published in Manning-Berg et al., 2022 from an excel model. The lab-based decomposition experiments of microbial mats and consortiums do seem to follow similar decomposition patterns as the monocultures did in the Manning-Berg et al., 2022 paper, which suggests that microbes in a community decompose similarly to individuals in a monoculture as opposed to highlights the way in which organisms are likely decaying over time.	**Budget and Schedule** Total Budget: $90,000.00 Actual Used: $90,000.00 Balance: $ 0.00 Total period of performance is 12 months. Task 1: months 1-12 Task 2: months 2-6 Task 3: months 7-8 Task 4: months 9-12 **Deliverables** • Final report detailing results, financials, and future work • Publication of the laboratory work (in prep) • External and internal conference presentation at UTC Research dialogs and GSA sectional and national meetings **Organization Information** *Department of Biology, Geology, and Environmental Science (Dept 2653)* *The University of Tennessee at Chattanooga* *Chattanooga, TN 37403* *423-425-4407* *Ashley-manning-berg@utc.edu*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Publish the decomposition pattern models of individual microbes	Published in January 2022
Perform a decomposition experiment on a microbial mat	A decomposition experiment of a microbial mat, cyanobacteria consortium, and green algae consortium was performed. Thanks to photos of a recently collected living mat (from colleagues at Johns Hopkins University and UC – Santa Barbara), a natural “starting” point for a microbial mat was documented as well.
Disseminate results of decomposition experiment (consortiums/communities not monocultures)	Both studies mentioned above have been presented at Research Dialogs, and the regional and national GSA meetings, and discussed during invited seminar talks.
Get a full copy of the code to create the microbial mat and be able to successfully run the model	I was able to get a copy of the code from the last group that published modifications to it. It was complete and successfully ran in the R-studio environment. Over the summer of 2022, I had a math student (finished MS degree) pull apart the model and identify each of the parameters. He was also able to get a biomass value for each layer of the microbial mat over a 36-hour period.
Incorporate the decomposition pattern models created through experimental taphonomic research into the mat model	I originally planned to use the biomass values from the model to inform a “starting biomass” for two of the decomposition models published in January of 2022. While trying to incorporate this data, it became apparent that using the biomass value to estimate taphonomic grades for decomposing mats repeated but did not add to the published models, which reported variation in terms of percent of the mat. It may still be possible, but I’m going to have to rethink the computer modeling aspect of the research.
Disseminate results	Results of the decomposition experiments have been shared at various conferences. These results will hopefully be replicated and then written into a Geobiology manuscript by the end of the year.

Challenges & Strategies Used to Address / Overcome:

The most significant barrier to this project was my lack of coding knowledge. Part of that challenge is that I'm not sure what information I need. I'm doing a lot of reading about modeling in biology (neither of these fields are my forte). To accommodate these barriers, I originally started the project with a Co-I from the SIMcenter. When that fell through, I worked with a math student between the summer he obtained a MS and started a PhD. This student was able to break the code, which I received from the last person to update it, into chunks and described what each chunk does in the model. He also identified the biomass results that were obtained from the model, and we explored whether the biomass concentration was a useful parameter to apply to decomposition. We ultimately decided that using biomass concentration as a parameter only mimicked the data presented in the model from Manning-Berg et al., 2022.

I'm happy with the laboratory data that has been collected. I have 15 weeks of data collected by an undergraduate student. We are in the process of writing up the manuscript, but external colleagues have encouraged me to have a second student repeat the process to verify that we are consistent in our taphonomic measurements and counts. I have an independent research student working on that during the fall of 2023.

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

I was not able to combine the actualistic lab experiments to the microbial mat model as I had hoped. R may not be the correct program to use if I want to incorporate actualistic studies into the model, given that there is a set death rate within the microbial mat that is unknown from lab experiments. It may be better to explore the modeling program PHREEQC, which has shown some promising results on microbial mat modeling in other studies.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

This research has allowed me (the PI), who is at the early career stage, to help establish a lab and present research at local and national conferences. The funding provided helped tremendously with purchasing supplies and equipment that I could not afford with my start-up funds and furnished most of the equipment in my lab. These funds allowed me to build a state-of-the-art microscope that until recently was the only microscope in the Southeast able to create photomicrograph mosaics that enable a user to investigate small-scale features within the larger image while being able to zoom-out rapidly to look at the overall fabric of the microbes or microbial mats. Without this funding, I would not be able to perform any aspect of my research at UTC. These funds allowed me to collaborate with existing colleagues and travel to their institutions to use analytical instruments my research requires, including The University of Tennessee – Knoxville, Gustavus Adolphus College, The University of Cincinnati, and the Jet Propulsion Laboratory. I was also able to expand my network of colleagues because of this funding and started to collaborate with researchers from The University of California at Riverside, Johns Hopkins University, and The University of California at Santa

Barbara. The funding allowed me to present these results at national conferences and stay connected in my field. My research has been presented at invited research talks at Vanderbilt University, The University of Missouri, The University of Cincinnati, the national Geological Society of America meeting in 2020, and Boise State University (in Fall of 2023).

Students Impacted

Elizabeth (Katee) Lam (seeking a B.S. in History) – Katee has growing microbial consortiums mats and monitoring decomposition. From this experience she has learned how to use the microscope and basic laboratory skills. She has presented her research at Research Dialogues and has been a co-author one 3 Geological Society of America (GSA) presentations- two national and one regional (funding limitations and class conflicts prevented her presenting at the conferences).

Matthew (Gage) Plott (just finished M.S. in Math) - Gage worked with the R code for me over the summer of 2022. He was able to compare the parameters listed in the published papers to the associated code and annotate the code for me. He also helped me to identify areas where I might want to make changes in the code (e.g., atmospheric concentrations for oxygen and CO2, and time steps for organism death within the modeled microbial mat). He also deciphered the biomass concentrations for several days after the initial spin-up of the model. The data provided a biomass value every 12 hours that I might be able to use for a starting biomass in other models.

Community and Broader Impacts

This is the first attempt to look at decomposing microbial mats. So far, the geobiology community has only investigated monocultures; largely because it is rare to see a microbial mat preserved in the rock record. Microbial organisms, however, live in larger communities and grow as one species benefits from the metabolic byproducts of the species above it. By investigating mat decay and the decomposition of microbial communities, we can get insight into whether the entire mat and its layers or fabric can be preserved, and if the lack of preserved microbial mats.

is the result of biologic decomposition or if it is more closely related to preservation processes (how the organisms are preserved) and potential (the likelihood they will be preserved because they lack hard parts). Understanding how these individuals and consortiums decompose or preserve will also inform how we look for potential extraterrestrial life in the Solar System, specifically Mars.

Scholarly Products

Publications:

- Lam, Elizabeth K., and Manning-Berg, Ashley R., Taphonomic changes of microorganisms within microbial communities (in prep). Geobiology (IF = 4.2)

External Conferences:

- Southeastern-Northcentral Geological Society Meeting (refereed conference)
  - Manning-Berg, Ashley R., **Lam, Elizabeth Kathleen**., 2022. Decomposition pathways of microbial communities and mats. Geological Society of America Abstracts with Programs. Vol. 54, No. 4, 2022doi: 10.1130/abs/2022NC-374872
- National Geological Society Meeting (refereed conference)
  - Manning-Berg, Ashley R., **Lam, Elizabeth Kathleen**., 2022. Taphonomic changes and decomposition pathways of microbial consortiums. Geological Society of America Abstracts with Programs. Vol 54, No. 5. doi: 10.1130/abs/2022AM-381907
  - Manning-Berg, Ashley R., **Lam, Elizabeth K.**, Riedman, Leigh Anne, Gomes, Maya. 2021. Modern microbial mat taphonomy and its implications on microfossil preservation. Geological Society of America Abstracts with Programs. Vol 53, No. 6. doi: 10.1130/abs/2021AM-371005

Presentations at UTC:

- Research Dialogs
  - Lam, Elizabeth, K., and Manning-Berg, Ashley, 2022. Qualifying changes to microbial communities during decomposition to interpret mat morphologies observed in the rock record. Research Dialogues UTC.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

By presenting this research at local and national conferences, I have been able to expand my network of people who I can ask for help now and continue to work with in the future. Although I continue to collaborate with colleagues at the Jet Propulsion Laboratory and Gustavus Adolphus College (Dr. Julie Bartley, 1 of 2 experts in the field of microbial taphonomy), I have also expanded my network of colleagues as she has worked with researchers from The University of California at Riverside (Dr. Gordon Love), Johns Hopkins University (Dr. Maya Gomes), The University of California at Santa Barbara (Dr. Leigh-Ann Reidman), and Pennsylvania State University (Dr. Erica Barlow).

I attended a workshop in the Bahamas to observe modern microbial mats living in a natural setting. Seeing mats in nature allowed me to form more hypotheses about preservation potential and get a more realistic view of decomposition patterns from large mats that have been active in this environment for 2310 ± 70 years.

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?

Over the next year I plan to continue actualistic lab experiments on microbial mats and communities. I will likely switch most of my research to using consortiums instead of monocultures to continue to observe changes at the community-scale. I hope to follow up this work with a student-lead publication, however, I will have a second student repeat the experiment to show consistency in the methodology.

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

I plan to apply for funding to look at the microbial mats preserved in Storr's Lake on San Salvador Island, Bahamas. These mats are modern, and despite containing some organisms that are not analogous to Precambrian microbes, I hope to perform a more robust "starting point" of decomposition for a microbial mat. This research will emphasize that although we are able to see a pattern of decomposition in microbial communities, it is important to consider that mat communities grow as a result of decomposition and the starting point of the decomposition models is not necessarily going to be at a taphonomic grade of Good.

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

Because of the decomposition experiments, one of my colleagues, Dr. Erica Barlow has reached out to ask if I can help her identify a preserved organism by comparing it to a decomposing example of the extant bacteria. A graduate student at Vanderbilt (Kelly Tingle) who is performing actualistic experiments has reached out to me for guidance on her PhD work.

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

A significant barrier is the modeling part of the project. I have not figured out how to change the code, and I’m not familiar with the R software. I also need to find a biologist who can use the programming software and understand the math required to incorporate decomposition parameters into the code.

FINANCIAL ACCOUNTING

N/A

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Hong Qin, Lead PI

Co-PI(s): Ziwei Ma, Azad Hossain
Other Personnel: None

Project Title: Addressing sampling bias in SARS-CoV-2

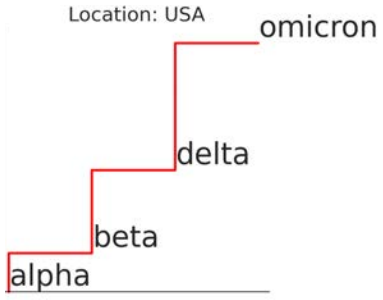
Date Submitted: Fall 2020

Award Start – End Date: July 1, 2021 – June 30, 2023 with no-cost extension

Non-Technical Summary:

This project provided timely support for us to explore solutions to address the sampling bias in the SARS-CoV-2 and develop quantitative models and computational methods to quantify the relative transmission potential of SARS-CoV-2 variants. During this project period, we won a $1M research grant from the National Science Foundation, published two peer-reviewed conference proceedings, and trained multiple graduate and undergraduate researchers. Scientifically, we have preliminary results to demonstrate the utility of our proposed differential population growth fitness for monitoring the SARS-CoV-2 variants, and how our deep learning neural network models can be used to analyze new viral sequences

PROJECT TITLE: "Addressing sampling bias in SARS-CoV-2"
Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
• Develop methods to accurately monitor and quantify the transmission of viral strains. • Quantify the transmission potentials of various viral strains.	• NSF, CCF 2200138, "PIPP Phase I: Develop and evaluate computational frameworks to predict and prevent future coronavirus pandemics". PI Qin, Co-PIs Choy, Zhang, Qingge, Ma. Senior personnel: Hossain, Zahry, Heath, Sistrunk. August 1, 2022-February 2024. $1M. • UTRF 23127, "A computational approach to predict pathogenic potential of viral pathogens from primary sequences".
RESULTS	**OTHER INFO**
 *Fitness Stair of Sars-CoV-2 estimated by our method.*	**Budget and Schedule** Total Budget: $90,000 Actual Used: $90,000 Balance: $0 Total period of performance is 12 months. Task 1: Months 1-9 Task 2: Months 10-24 (extended) **Deliverables** • UTRF IP disclosure 23127 **Organization Information** *University of Tennessee at Chattanooga*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Aim 1. Compare a suite of parametric and non-parametric methods to address the sampling biases of SAR-CoV-2 sequences. Specifically, we will resample genotypes using equidistant quantile matching with observed COIVD-19 cases temporally and spatially. We will investigate a three-parameter skew normal distribution to correct outliers, a more generalized skewed t-distributions, and gamma distribution. We will benchmark the performance using sequencing uncertainties and simulated data.	We performed resampling methods and used the resampled data for machine learning training and fitness estimation.
Aim 2: Accelerate resampling, permutation, and GWAS for SARS-CoV-2 using distributed and parallel computing. We will use cluster computing methods and tensor-flow GPU-acceleration to improve the permutation performance for large scale GWAS for SARS-CoV-2.	We compared the performance of deep learning and GWAS on SARS-CoV-2 classification.
Aim 3. Prototype a semi-automatic pipeline to monitor genotypes and environmental measurements for SARS-CoV-2. We will automate the scripts to curate weather conditions associated with genotypic changes in SARS-CoV-2 genomes. We will visualize the GWAS analyses through an ArcGIS dashboard	A GIS dashboard was built.

Challenges & Strategies Used to Address / Overcome:

None.

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

None

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

PI Hong Qin was recently promoted to a tenured full professor and department Head.

Students Impacted

Landen Bauder, MS student

Connor Firat, MS student

Parisa Hatami, Ph.D. student

Gertrude Osei, MS student

Braxton Anzalone, BS student.

Community and Broader Impacts

Dr. Qin organized and taught a Python bootcamp for 18 K12 teachers and a high school bootcamp to 6 African American students in the summer of 2022. Some of the projects were used for REU researchers in the summer of 2022.

Scholarly Products

Publications:

- None in the no-cost extension period.

External Conferences:

- None in the no-cost extension period.

Presentations at UTC:

- None in the no-cost-extension period.

Inventions or Other Intellectual Property

UTRF Invention 23127 was disclosed.

Research Outreach & Collaboration

None in the no-cost extension year.

EXTERNAL FUNDING

Proposal Submissions

None in the no-cost extension period.

Contracts/Awards Received

NSF, CCF 2200138, “PIPP Phase I: Develop and evaluate computational frameworks to predict and prevent future coronavirus pandemics”. PI Qin, Co-PIs Choy, Zhang, Qingge, Ma. Senior personnel: Hossain, Zahry, Heath, Sistrunk

Sponsored Program Capacity Building Activities

None in the no-cost-extension period.

WHAT’S NEXT FOR THIS RESEARCH?

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

We plan to apply for more external grants.

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

We plan to apply for more external grants.

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

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

FINANCIAL ACCOUNTING

N/A

Fiscal Year 2022 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Reetesh Ranjan, Lead PI

Co-PI(s):
Other Personnel:

Project Title: "Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy"
Date Submitted: 7/30/2021

Award Start – End Date: July 1, 2020 – June 30, 2021

Non-Technical Summary: Numerical investigation of stratified turbulent flows observed in engineering and geophysical flows is challenging due to the added complexity of the effects of stratification on turbulence. The challenges are increased further in the flows where differential diffusion effects are present due to the dependence of density stratification on temperature and salinity through a nonlinear equation of state (EoS). Large-eddy simulation (LES) is a computationally tractable approach for the investigation of such flows at practically relevant conditions. However, the subgrid-scale (SGS) closures used in LES need to be robust and accurate to account for the effects of stratification on the subgrid processes. The research carried out under this effort addressed several aspects of the challenges associated with the modeling of differential diffusion effects in these flows. First, it examined the effects of moderate levels of differential diffusion at moderate Reynolds number (*Re*) through direct numerical simulations, where the role of linear and nonlinear EoS was also characterized. Secondly, a generalized hybrid multi-scale model leveraging the accuracy of the two-level simulation (TLS) model and the efficiency of the LES model is established for physics-based efficient modeling of stratified turbulence. The established model is used to study features of high *Re* axisymmetric towed wake at realistic flow conditions. A deep neural network-based data-driven modeling strategy has been implemented to assess its capabilities in comparison to physics-based models for LES of wall-bounded turbulent flows. Finally, proper orthogonal decomposition and dynamic model decomposition-based tools have been established to examine the fundamental aspects of stratified turbulence.

The research effort during the period of performance has supported 1 ongoing MS thesis-related research, 2 MS independent studies, 3 international conference presentations, 2 international conference articles, 2 internal conference presentations, and 2 journal articles that are currently being prepared. The project has also trained 3 graduate students on simulation, modeling, and analysis of turbulent combustion by using high-performance computing (HPC) resources at UTC. The project has demonstrated the use of HPC resources facilitated by the CEACSE at UTC. So far, under the project, one pre-proposal and one invited proposal have already been submitted to external agencies and further white papers and proposals will be submitted in the following year.

PROJECT TITLE: Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy

Technology Area of Interest: Aerospace, Defense, and Energy Applications

TECHNICAL APPROACH

- DNS of stratified turbulence with nonlinear equation of state (EoS) and differential diffusion effects
- Extend two level simulation (TLS) model to account for density stratification
- Develop tools for statistical, spectral, and modal analysis of stratified turbulent flows
- Assess deep neural network based data-driven model for LES of wall-bounded turbulent flows
- DNS and LES of periodic channel and towed wake under neutral and varying level of density stratification

OUTCOMES

- Fundamental investigation of effects of differential diffusion and nonlinear EoS on stratified turbulence
- Extended TLS and hybrid TLS-LES models for stratified turbulent flows and DNN based model for LES of wall-bounded turbulent flows
- Trained 3 graduate students on simulation of turbulent flows using HPC tools and analysis of results using Python, Tecplot
- Supported 1 ongoing MS thesis, 2 international conference article, 3 international conference presentations, 2 internal conference presentations, 2 journal articles under preparation, and 2 white papers/proposals.

RESULTS

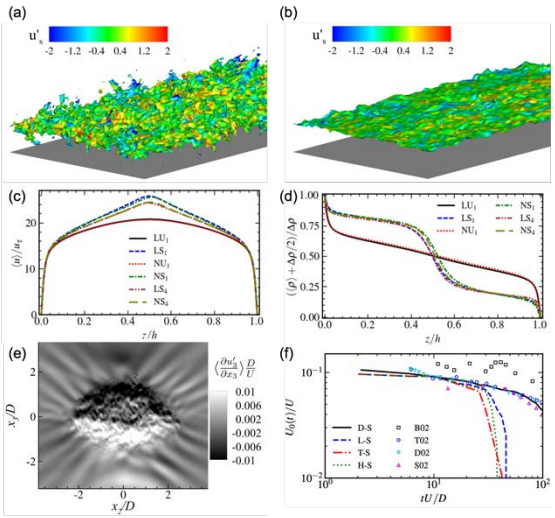


Figure 1 Iso-surface of density under neutral (a) and stratified conditions demonstrating suppression of vertical mixing under stable stratification, vertical variation of mean streamwise velocity (c) and mean density (d) comparing neutral (LU_1 and NU_1) and stratified cases (LS_1, NS_1, LS_4, NS_4) with the effects of differential diffusion (LS_4 and NS_4) and nonlinear EoS (NU_1, NS_1, NS_4), internal waves in stratified towed wake flow (e), and time evolution of peak defect velocity in stratified towed wake flow comparing DNS, LES, hybrid TLS-LES with reference numerical and experimental results (f).

OTHER INFO

Budget and Schedule

Total Budget:	$93867.00
Actual Used:	$44542.66
Balance:	$49324.34

Total period of performance is 12 months with multiple tasks spread out during the entire year.

Deliverables

- Quarterly 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 presentations

Organization Information

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ACCOMPLISHMENTS & OUTCOMES

Project Overview

Stably stratified turbulent flows are observed in several engineering, geophysical, and environmental flow systems, and therefore, the study of such flows is of great interest to hydrogeologists, oceanographers, and atmospheric and naval researchers. Numerical investigation of such flows is challenging because of the additional complexities introduced by the presence of stratification on turbulence. In the subsurface naval flows, where the density of the water is dependent on the temperature and the salinity of the water, the presence of a differential molecular diffusion of the temperature and salinity fields makes the numerical investigation computationally prohibitive due to the need to capture a wide range of scales. Additionally, the dependence of density on temperature and salinity through a nonlinear equation of state (EoS) furthers the complexity of the physical processes in such flows. Although direct numerical simulation (DNS) allows for studying fundamental aspects of such flows, its high computational cost limits its applicability to low to moderate Reynolds number (*Re*) flows in simpler configurations. To this end, large-eddy simulation (LES) presents a viable approach, where the effects of unresolved scales are modeled through subgrid-scale (SGS) closures. However, such closures need to be robust to account for processes associated with the stratified turbulence. In this research project, an investigation of fundamental aspects of the effects of differential diffusion and the role of types of EoS on stratified turbulence through DNS has been carried out. In addition, a computationally efficient hybrid multi-scale model and a data-driven model for the LES of such flows have also been established in this project.

The activities carried out under this project have resulted in computational tools, modeling capabilities, and analysis tools, which can be used to examine stratified turbulent flows in canonical and practically relevant configurations. These activities have demonstrated the capabilities within the research group of the PI to carry out research in the broader area of simulation and modeling of stratified turbulent flows. The project has also broadened the capabilities of CEACSE at UTC in conducting simulation-based investigations of relevance to aerospace, defense, and energy applications. The project has trained both graduate and undergraduate students in the use of HPC tools to solve fundamental and applied problems pertaining to naval flows. The project accomplishments in the form of computational capabilities, publications, and presentations will allow the PI to work on proposals seeking external funding.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Examine effects of differential diffusion and EoS	DNS of six cases was performed to examine fundamental aspects of stratified turbulent channel flows and to understand the effects of differential diffusion and linear vs nonlinear EoS. A comprehensive study using statistical, spectral, and modal analysis tools was performed.
TLS model for stratified flows	Implemented the TLS model to enable its application to stratified turbulent flows.

Demonstrate hybrid multi-scale strategy	Assessed capabilities of the hybrid TLS-LE strategy by performing simulation of axisymmetric towed wake under neutral and stratified conditions
Study features of stratified towed wake	Compared instantaneous and statistical results pertaining to stratified wake demonstrating the strengths and limitations of hybrid TLS-LES strategy
Implement data-driven model for LES	Deep neural network-based model for subgrid stress was implemented in the solver and demonstrated by simulating smooth and rough, turbulent channel flows.

Challenges & Strategies Used to Address / Overcome:

A major challenge was related to working with students who had limited experience with code development. However, a hands-on training experience, collaborative working environment, and weekly reporting from students helped me to address this challenge. An additional challenge was associated with hiring graduate students for this project. The PI was not able to find graduate students for this project till the start of Spring 2023, which required the PI to work on several aspects of the project in the Fall 2022 semester.

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

Initially, I had the expectations that the graduate students would be able to contribute to some of the key code development activities. However, a significant amount of training was needed before students were able to contribute to some of the code development activities. The rest of the code implementation was carried out by the PI.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The research work carried out under this effort will have impacts at various levels on the career of the PI in the area of computational modeling of stratified turbulent flows pertinent to naval applications. It has allowed establishing a computational framework, which can be used to carry out fundamental and applied studies of stratified turbulence. The computational strategy demonstrated under this research has established accurate and efficient approaches for simulation of passive/active scalar transport, which is key for the prediction of features of stratified turbulence. It has further extended the collaborative research work with the researchers from

Georgia Tech. The data-driven modeling strategy implementation has demonstrated the availability of machine learning tools for LES within the PI research group. The high-fidelity simulations conducted during this project have demonstrated the HPC-based modeling and simulation capabilities with the PI's research group. Overall, the resulting computational capabilities, publications, and presentations are helpful to the PI in seeking extramural funding.

Students Impacted

1. **Steven Thompson** (MS with thesis option, Expected Graduation in Summer 2024)**:** Mr. Thompson learned to carry out high-fidelity simulations of stratified turbulence using HPC resources. Additionally, he learned the skills to analyze large-scale datasets generated from simulations using Python. A key focus was to analyze statistical, structural, spectral, and modal aspects of stratified turbulence. He has been trained in the usage of tools such as MINCLES solver, Tecplot, Paraview, Python, GitHub, Latex, Trac, and POD/DMD tools. He worked on this project in Fall 2022 as an undergraduate researcher before switching to MS in Spring 2023.
2. **Amin Amiri** (MS, Expected Graduation in Summer 2024)**:** Mr. Amiri was trained to carry out high-fidelity simulation using HPC resources. He implemented data-driven based pre-processing scripts using TensorFlow software and LES model relying on deep neural network for simulation of wall-bounded turbulent flows.
3. **Robert Smith (**MS, Expected Graduation in Summer 2024): Mr. Smith has worked on implementing modules for performing simulation of forced isotropic turbulence.
4. **Nelson Rainey** (UG, Graduated in Fall 2022): Mr. Rainey was trained on the usage of HPC tools and performing simulations of stratified wake flows.

Community and Broader Impacts

The research carried out during the period of performance addressed several challenges associated with modeling and simulation of stratified turbulent flows, which are of relevance to underwater naval applications. It has assisted in extending the expertise of the PI in the area of multi-scale modeling of turbulent flows w/o active/passive scalar transport. The demonstration of the novel hybrid modeling strategy has enabled a robust approach for a community of researchers. The research project has also trained students in the use of advanced computational models and HPC resources for solving challenging problems in the area of turbulent flows with density stratification, and passive/active scalar mixing. The research has also featured the use of HPC resources at UTC and has extended the scope of capabilities offered by the CEACSE at UTC to the external agencies. Finally, the resulting computational capabilities, presentations, and publications will assist the PI in seeking extramural funding.

Scholarly Products

Software:

1. MINCLES: Incompressible flow solver with DNS and LES capabilities for wide range of turbulent flows
2. POD/DMD/ANN tools: In-house tools to perform POD/DMD analysis and pre-processing of ANN-based LES closures.

Publications:

2. A. Amiri, E. Durant, and R. Ranjan, “Subgrid modeling using deep neural networks for simulation of smooth and rough turbulent channel flows”, AIAA-2023-3973.
3. S. Thompson, and R. Ranjan, “On the effects of differential diffusion and equation of state in stably stratified turbulent channel flow”, APS, DFD, 2022.
4. R. Ranjan, S. Kim, & R. Ranjan, “Hybrid Two-Level and Large-Eddy Simulation of the Wake of a Towed Sphere in Stably Stratified Fluid”, 34th Symposium on Naval Hydrodynamics, 2022.
5. S. Thompson, and R. Ranjan, “On of the effects of differential diffusion and equation of state in stably stratified turbulent channel flow”, Under Preparation for Journal Submission, 2023.
6. A. Amiri, E. Durant, and R. Ranjan, “Subgrid modeling using deep neural networks for simulation of smooth and rough turbulent channel flows”, Under Preparation for Journal Submission, 2023.

External Conferences:

- Subgrid modeling using deep neural networks for simulation of smooth and rough turbulent channel flows, AIAA Aviation Forum and Exposition, 2023 (Presenter: R. Ranjan).
- On the effects of differential diffusion and equation of state in stably stratified turbulent channel flow, APS DFD, 2022 (Presenter: S. Thompson).

Presentations at UTC:

- A. Amiri, and R. Ranjan, “Investigation of Reinforcement Learning in Subgrid-Scale Modeling in Large Eddy Simulation”, Spring Research and Arts Conference, UTC, 2023 (Presenter: A. Amiri).
- S. Thompson, and R. Ranjan, “Numerical Investigation of Physical and Modal Characteristics of Stably Stratified Turbulent Channel Flow”, Spring Research and Arts Conference, UTC, 2023.

Inventions or Other Intellectual Property

In-house research code: MINCLES

Research Outreach & Collaboration

The research conducted under this effort has extended the collaboration with Georgia Tech researchers.

EXTERNAL FUNDING

Proposal Submissions

Numerical Investigation and Multi-Scale Modeling of Differential Diffusion Effects in Stably Stratified Turbulent Flows, Invited Proposal, CHL-10 ERDC, 2023.
Numerical Investigation and Multi-Scale Modeling of Differential Diffusion Effects in Stably Stratified Turbulent Flows, Accepted Pre-Proposal, CHL-10 ERDC, 2022.

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?

The PI is working on completing the journal paper submissions. In addition, the PI will be submitting white papers and proposals, which will leverage the accomplishments of the project. In particular, the PI is planning to pursue three research directions in the next few years. These include (a) fundamental investigation of differential diffusion effects in wake flows, (b) application of hybrid TLS-LES to simulate wall-bounded and wake flows, and (c) extension of data-driven models for simulation of stratified turbulence.

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

The work carried out under this research project has further established the ongoing collaboration of the PI with the researchers from Georgia Tech, which will be extended further in future. The goal of future collaborations will be on to incorporate features of machine learning techniques, GPU computing to further enhance the efficiency of the current computational models and techniques, and to develop analysis tools for spectral POD to examine internal waves in stratified turbulent flows.

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

The PI did not experience any budget issues during the project. The project was extended in December 2022 for a year due to the non-availability of graduate students for this project. However, the extension was withdrawn in Spring 2023 with leftover funds. The leftover funds for this project after the period of performance have been taken over by the UTC Research Institute.

Fiscal Year 2022 Final Project Report –

For Grants authorized to continue into FY 2023

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Reetesh Ranjan, Lead PI

Co-PI(s): N/A
Other Personnel: N/A

Project Title: "Modeling of Transition to Turbulence in Large Eddy Simulation Using the Two-Level Simulation Approach"

Date Submitted: 8/28/2022

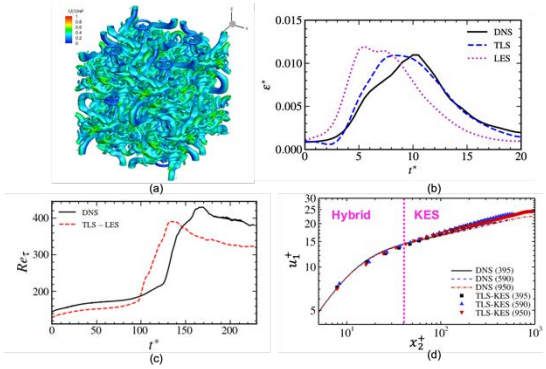
Award Start – End Date: July 1, 2021 – June 30, 2023

Non-Technical Summary: Transition to turbulence is observed in several aerodynamic applications such as turbomachinery and flow past aircraft wings. Specifically, in wall-bounded flows, transition affects the skin friction coefficient, the wall heat flux, and the spectral and spatio-temporal characteristics. Therefore, an accurate prediction of the onset of transition and the corresponding flow features is important from the aerodynamic design perspective. The presence of such flow complexities makes the numerical investigation of transitional flows extremely challenging. While direct numerical simulation (DNS) can be used to examine fundamental features of such flows, large-eddy simulation (LES) tends to be more suitable for the investigation of practical applications. However, models for LES are usually derived for fully developed turbulence, thus requiring improved or alternate strategies. The research effort in this project assessed a hybrid modeling strategy for LES of transitional flows where the two-level simulation (TLS) model, a multi-scale model, is used for near-wall modeling. TLS model does not employ the notion of eddy viscosity, which allows it to capture small-scale physics such as anisotropy, vorticity dynamics, backscatter, and co-/counter-gradient transport. The hybrid modeling strategy was assessed through a series of well establish test cases, and it was demonstrated that the hybrid model can capture the relevant flow physics during the transition in wall-bounded flows.

The research effort during the period of performance has resulted in 1 MS thesis, 3 international conference presentations, 2 international conference articles, 2 internal conference presentations, and 1 journal article that is currently being prepared. The project has also trained 2 graduate students and 1 undergraduate student on simulation, modeling, and analysis of wall-bounded transitional and turbulent flows by using high-performance computing (HPC) resources at UTC. The project has demonstrated the use of HPC resources facilitated by the CEACSE at UTC. So far, under the project, one white paper and two proposals have already been submitted to external agencies and further white papers and proposals will be submitted in the following year.

PROJECT TITLE: "Modeling of Transition to Turbulence in Large Eddy Simulation Using the Two-Level Simulation Approach"
Technology Area of Interest: Aerospace, Defense, and Energy Applications

TECHNICAL APPROACH	OUTCOMES
• Generalize the hybrid TLS-LES strategy to make it modular, which will allow blending of the TLS model with different LES closures. • Conduct DNS cases for the Taylor-Green vortex flow and temporal transition in a channel so that they can be used as reference datasets for assessment of different modeling techniques. • Carryout verification and validation studies to assess the performance of the generalized hybrid TLS-LES strategies. • Improve LES strategies by utilizing the TLS-SS data in the transitional regime. • Perform further studies by using the established hybrid TLS-LES strategy simulate spatial transition.	• Established tools and models for simulation of transition to turbulence • Trained 2 graduate students and 1 undergraduate student on simulation of wall-bounded transitional and turbulent flows using HPC tools and analysis of results using Python, Tecplot, Paraview • Resulted into 1 MS thesis, 2 international conference article, 3 international conference presentations, 2 internal conference presentations, 1 journal article under preparation, 1 white paper and 1 proposal.

RESULTS	OTHER INFO
 *Figure 2 Vortical structures in the Taylor-Green vortex flow in post-transition regime (a), comparison of kinetic energy dissipation rate obtained using LES and TLS models with the reference DNS (b), time evolution of frictional Reynolds number illustrating laminar-to-turbulent transition obtained using the TLS model and compared with reference DNS (c), mean streamwise velocity in a channel obtained using hybrid TLS-KES model and compared with reference DNS (d).*	**Budget and Schedule** Total Budget: $89675.00 Actual Used: $88686.90 Balance: $988.10 Total period of performance is 12 months with multiple tasks spread out during the entire year. **Deliverables** • Quarterly 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 presentations **Organization Information** *Department of Mechanical Engineering* *University of Tennessee at Chattanooga* • *615 McCallie Ave, Chattanooga, TN 37403* *Phone: 423-425-4017, Email: reetesh-ranjan@utc.edu*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Transition to turbulence is observed in several aerodynamic applications such as turbomachinery and flow past aircraft wings. Specifically, in wall-bounded flows, transition affects the skin friction coefficient, the wall heat flux, and the spectral and spatio-temporal flow characteristics. Therefore, an accurate prediction of the onset of transition and the corresponding flow features is important from the design, control, and optimization perspective. The presence of such flow complexities makes the numerical investigation of transitional flows extremely challenging. While direct numerical simulation (DNS) can be used to examine fundamental features of such flows, large-eddy simulation (LES) tends to be more suitable for the investigation of practical applications. However, models for LES are usually derived for fully developed turbulence conditions, thus requiring either improved or alternate strategies. The research effort in this project assessed a novel hybrid modeling strategy for LES of transitional flows where the two-level simulation (TLS) model, a multi-scale approach, is used for near-wall modeling. In the TLS model, scale decomposition is used (as opposed to filtering used in LES), and both the large-scale (LS) and a modeled version of the small-scale (SS) fields are simulated and then combined to recover the full flow field without using the notion of eddy viscosity. Past studies have shown that the TLS model can predict SS physics such as anisotropy, vorticity dynamics, backscatter, and co-/counter-gradient transport in high Reynolds number turbulent flows. Also, advanced modeling strategies for LES in regions away from the wall have been examined for their capabilities, which include, the algebraic integral length scale approximation (ILSA) model, the one-equation locally dynamic kinetic energy model (LDKM), and the two-equation kinetic eddy simulation (KES) model. The hybrid modeling strategy has been assessed through a series of well establish test cases that exhibit a temporal transition from laminar to turbulence state. These cases include the Taylor-Green vortex (TGV) flow and the periodic channel flow.

In this project, three different computational tools have been developed further. These include the well-established incompressible flow solver referred to as MINCLES solver, the Orr-Sommerfeld equations solver referred to as OS-Solver, and the extended version of OpenFOAM software referred to as UTCFOAM solver. The TGV flow was simulated using the MINCLES solver with a specified initial condition for the flow field. For the transition within a periodic channel configuration, specific disturbances to the initial velocity field are imposed to enable the transition from laminar to turbulence state by numerically solving the Orr-Sommerfeld equations and obtaining the unstable modes. The advanced algebraic, one-equation, and two-equation models for LES have been examined using both MINCLES and UTCFOAM solvers.

The activities carried out under this project have resulted in computational tools, modeling capabilities, and analysis tools, which can be used to examine laminar to turbulent transition within wall-bounded flows. These activities have demonstrated the capabilities within the research group of the PI to carry out fundamental and applied research in the broader area of simulation and modeling of wall-bounded turbulent flows. The project has also broadened the capabilities of SimCenter at UTC in conducting simulation-based studies of relevance to aerospace, defense, and energy applications. The project has trained both graduate and undergraduate students in the use of HPC tools to solve fundamental and applied problems pertaining to turbulent flows. The project accomplishments in the form of computational capabilities, publications, and presentations will allow the PI to work on proposals seeking external funding.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Establish the TLS model for transitional flows	The TLS model was evaluated for its abilities to predict the laminar-to-turbulent transition. Both a priori and posteriori assessment studies were performed by considering two canonical test cases, which include the TGV flow and the periodic channel flow.
Demonstrate capabilities of hybrid TLS-LES model	The hybrid TLS-LES modeling strategy was assessed for its capabilities in the simulation of transitional flows. In additional hybrid TLS-LES models with advanced LES models in the regions away from the wall and TLS as a near-wall model was examined. These advanced LES models included the ILSA, LDKM, and KES models.
Investigate characteristics of boundary layer transition	The hybrid TLS-LES model was evaluated for its ability to capture spatial transition over a flat plate.
Improve closures from TLS-SS data	A mixed model strategy is being evaluated by blending a conventional algebraic model with the stochastic term relying on the TLS-SS data that can capture subgrid physics such as backscatter, counter-gradient transport, non-equilibrium, etc.

Challenges & Strategies Used to Address / Overcome:

A major challenge was working with students who had limited or no experience with computational tools. However, a hands-on training experience, collaborative working environment, and weekly reporting from students helped me to address this challenge.

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

Initially, I had expectations that the graduate student would be able to contribute to some of the code development activities. However, a lack of experience made it challenging leading me to adjust the task assignments.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The research work carried out under this effort will have impacts at various levels on the career of the PI in the area of modeling and investigation of wall-bounded turbulent flows. It has allowed the establishment of a computational framework, which can be used to carry out fundamental and

applied investigation of laminar-to-turbulent transition typically observed in several aerodynamic applications. The computational strategy demonstrated in this research has established a hybrid multi-scale modeling strategy that can be used for an accurate and efficient simulation of transitional flows. The research work has further extended the collaborative work with the researchers from UTC and Georgia Tech. Furthermore, the high-fidelity simulations conducted during this project have demonstrated the HPC-based modeling and simulation capabilities with the PI's research group. Overall, the resulting computational capabilities, publications, and presentations are helpful to the PI in seeking extramural funding.

Students Impacted

1. **Mickael Young** (MS with thesis option, Fall 2022)**:** Mr. Young learned to carry out high-fidelity turbulent flow simulations using HPC resources. Additionally, he learned the skills to analyze large-scale datasets generated from simulations using Python. He also implemented a MATLAB-based solver for the Orr-Sommerfeld equations, which was key to the research project. His key focus was to carry out simulations of transitional flows and analyze statistical, structural, and spectral aspects of such flows. He has been trained in the usage of tools such as TLSLES solver, Tecplot, Paraview, Python, GitHub, Latex, Trac, and Cantera. He has contributed to two conference presentations, one conference article, one poster, and one UTC conference.
2. **Eli Durant** (MS, expected graduation Fall 2023)**:** Mr. Durant has learned several skills ranging from pre- to post-processing and running the simulations using HPC resources provided by SimCenter. He has learned tools such as Python, UTCFOAM, Tecplot, Paraview, Pointwise, Trac, etc. He has been trained in understanding the physics of wall-bounded turbulent flows. He has contributed to a conference presentation, a conference article, a poster, and a UTC conference.
3. **Robert Smith** (Undergraduate, graduated Fall 2022): Mr. Smith has learned to run the simulations using HPC resources provided by SimCenter. He has also learned tools such as Python, UTCFOAM, Tecplot, Paraview, Pointwise, Trac, etc. He has been trained specifically on mesh generation and post-processing of simulation results. He has contributed to a conference presentation, a poster, and a UTC conference.

Community and Broader Impacts

The research carried out during the period of performance addresses challenges associated with the modeling of laminar-to-turbulent transition, which is of great importance to aerospace and defense applications. The research work has an impact at various levels. It has helped extend the expertise of the PI in modeling and investigating wall-bounded transitional flows. The demonstration of the hybrid modeling strategy has led to an accurate, efficient, and robust approach for investigating such flows, which can lead to external collaborative research. The research has also trained students in advanced computational models and HPC resources for solving challenging problems in wall-bounded transitional and turbulent flows. The research has also featured the use of HPC resources facilitated by the SimCenter at UTC and has extended the scope of computational capabilities offered by the SimCenter to external agencies. Finally, the resulting computational capabilities, publications, and presentations will be helpful to the PI in seeking extramural funding.

Scholarly Products

Software:

1. MINCLES: An incompressible flow solver with multi-scale modeling capabilities

2. UTCFOAM: In-house and extended version of OpenFOAM
3. OS-Solver: A MATLAB based solver for Orr-Sommerfeld equation.
4. *Publications:*
5. M. Young, “Modeling of laminar-to-turbulent transition using a hybrid multi-scale simulation strategy”, MS Thesis, UTC, 2022.
6. E. Durant, M. Young, and R. Ranjan, “Hybrid Two-Level and Kinetic-Eddy Simulation Model for Numerical Investigation of Wall-Bounded Turbulent Flows”, AIAA-2022-3328, 2022.
7. R. Ranjan, “Large-Eddy Simulation of Transition to Turbulence using the Two-Level Simulation Approach”, AIAA-2021-2892, 2021.
8. M. Young and R. Ranjan, “Large-Eddy Simulation of Laminar to Turbulent using the Two-Level Simulation Approach”, In Preparation, 2022.

External Conferences:

- Two-Level Simulation of Transition to Turbulence in Wall-Bounded Flows, APS Division of Fluid Dynamics, 2021. (Presenter: M. Young)
- Hybrid Two-Level and Kinetic-Eddy Simulation Model for Numerical Investigation of Wall-Bounded Turbulent Flows, AIAA Aviation Forum and Exposition, 2022. (Presenter: E. Durant)
- Large-Eddy Simulation of Transition to Turbulence using the Two-Level Simulation Approach, AIAA Aviation Forum and Exposition, 2021. (Presenter: R. Ranjan)

Presentations at UTC:

- Hybrid Two-Level Large-Eddy Simulation of Transition to Turbulence, Research Dialogues, UTC, 2022 (Presenter: M. Young).
- Simulation of Laminar-to-Turbulent Transition using Two Level Simulation Model, CECS Tech Symposium, UTC, 2022 (Presenter: M. young).

Inventions or Other Intellectual Property

In-house research codes: OS-Solver, MINCLES, UTCFOAM

Research Outreach & Collaboration

The research conducted under this effort has extended the collaboration with Georgia Tech researchers and has led to a newer collaboration with Dr. Kidambi Sreenivas from UTC.

EXTERNAL FUNDING

Proposal Submissions

1. Towards Physics-Based Modeling of Transition to Turbulence in Wall-Bounded Flows with Predictive Capabilities, NSF CAREER, 2022 and 2023.

2. Study of Temperature and Three-Dimensional Effects on the Characteristics of Shock-Wave Turbulent Boundary Layer Interaction Using a Novel Hybrid Multi-Scale Modeling Strategy, DEPSCOR, 2021.

Contracts/Awards Received

None

Sponsored Program Capacity Building Activities

- Attended NSF CAREER proposal writing webinar, 2022.
- Discussion with ONR Program Manager, 2022.

PLAN FOR COMPLETION DURING THE NEXT FISCAL YEAR (EXTENSION PERIOD)

While most of the stated objectives of the project have been accomplished, some analysis work is currently underway. In addition, a journal article is currently being prepared, which will be the major focus during the extension period.

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 is working on completing the journal paper submission resulting from the work during this project. In addition, the PI will be submitting white papers and proposals, which will leverage the accomplishments of the project. In particular, the PI is planning to pursue three research directions in the next few years. These include (a) fundamental investigation of controlled spatial transition to turbulence, (b) application of the multi-scale model for capturing the physics of transition, and (c) investigation of transition within high-speed flows.

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

The work carried out under this research project has further established the ongoing collaboration of the PI with the researchers from Georgia Tech and researchers within the department at UTC, which will be extended further in the future. The goal of future collaborations will be to develop models for RANS-based studies of transition, leveraging GPU computing to further enhance the efficiency of the current computational models and techniques, and to investigate transition within high-speed aerodynamic applications.

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

The PI did not experience any budget issues during the project.

Fiscal Year 2021 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition

Sungwoo Yang, Lead PI

Co-PI(s): N.A.
Other Personnel: N.A.

Project Title: “A low-cost, passive solar process heat system”

Date Submitted: 06/30/2021

Award Start – End Date: July 1, 2020 – June 30, 2022 (1 year extended)

Non-Technical Summary:

Process heating constitutes nearly 70% of the total process energy consumed in the U.S. manufacturing sector, which is almost entirely extracted from fossil fuels. The demand for heating is particularly important for the food processing and beverage industry which consumes 340 TBtu produced using natural gas annually for process heating. Solar thermal energy is an ideal natural gas substitute for heat generation in the food processing industry. However, the high-cost and complexity of existing concentrated solar-powered industrial process heat systems have prevented their widespread adoption in food processing plants. We propose a low-cost, passive solar process heat system capable of reaching high temperatures and pressures (up to 200 °C, 15 bar) without the need for expensive solar tracking concentrators. The key technological innovation which enables our flat-plate type solar receivers to reach relatively high temperatures relevant for the food processing industry (100-200 °C) is the optically transparent, thermally insulating monolithic silica aerogel developed in our lab. These novel aerogel layers allow transmission of >96% incident solar energy while minimizing heat losses, resulting in efficiencies as high as 75% even without solar concentration.

The project experienced a lack of student researchers due to COVID-19. However, we were able to complete a few proposed milestones: (1) We finalized synthetic method of OTTI aerogel that demonstrated high transmittance (95% solar-weighted). (2) We synthesized ambiently dried aerogel that demonstrated ~ 90% transmittance that is equivalent to the best literature value. As the project is extended, we plan to further improvement. (3) We are in progress of developing optical and thermal computational modeling using RTE and Mie theory. (4) We built a lab-scale solar receiver. The PI plans to hire two PhD students to continue this project by using the rollover fund. The goals for the following years are to bring these threads together for research publications and external funding. The PI plans to continue to build a device-level prototype to demonstrate the viability of this approach. The PI plans to submit journal papers including patents. The research progress and products will allow the PI to pursue large funding opportunities, namely the National Science Foundation Faculty Early Career Development (NSF CAREER) award. These research activities are expected to increase the PI’s capacity to successfully compete for tenure.

PROJECT TITLE: “A low-cost, passive solar process heat system”
Technology Area of Interest: Energy Thrust

TECHNICAL APPROACH	OUTCOMES
The major milestones include 1. Finalized synthetic method of OTTI aerogel 2. Optimizing chemical recipes for ambiently dried aerogel 3. RTE and Mie theory modeling 4. Building solar collector assembly 5. Solar process heat generator design & modeling	The research outcomes include 1. Won Ruth S. Holmberg Grant 2. Submitted an NSF-ERI proposal, $200k (in review) 3. In progress (~50%), a peer-reviewed publication on ambiently-dried aerogel 4. Oral presentation at the Solar Energy Systems Conference (2021)
RESULTS	**OTHER INFO**
Please, see the attached research report for the details	Fill in your info below. **Budget and Schedule** Total Budget: $86,771.00 Actual Used: $36,167.00 Balance: $50,604.00 **Deliverables** • External funding proposal (submitted) • Final report detailing results, financials, and future work (submitted and there will be one more final report after the extended year) • Publication (in progress) • External and internal conference presentation (accepted at Solar Energy Systems Conference (2021)

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Chemical recipe for OTTI aerogel	Completed
Optimizing ambiently-dried aerogel	Fabricated. In progress for further improvement
Computational device design optimization	In progress (delayed)
Building solar receiver prototypes	Delayed due to COVID-19. But a lap-scale solar receiver built. Plan to build a larger system for outdoor experiment

Challenges & Strategies Used to Address / Overcome:

Followed are the challenges and strategies associated with the proposed project:

1. Developing collaboration: The PI aims to develop a novel chemical precursor to synthesize ambiently dried aerogel, which requires deeper chemical understanding. The PI is in progress developing collaboration with faculty members in the Chemistry department at UTC.
2. Limited researcher power: the proposed project requires significant amont of efforts to conduct various experiments and theoritical modeling. → Limited researcher power was major challenge the PI has been facing. Especially, due to COVID-19, it was extremely difficulty to keep researchers. As results, the several milestones were delayed. But, the PI plan to hire two PhD students using the carry over fund for the upcoming semester.

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

As a R3 institute, I found CEACSE grant is the most important grant that I can utilize to increase our research capability. Due to the unexpected delay, we were not able to complete all milestones, but plans to complete all in the upcoming semester. I was able to obtain several critical research developments with the CEACSE grant. Using these preliminary results, I have submitted multiple proposals and plan to submit more proposals to attract external funding. I really appreciate the CEACSE grant and the supporting team.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

With preliminary data, the PI plans to pursue external funding opportunities related to solar energy harvesting and energy-efficient building applications including NSF, NASA, ARPA-e, DARPA etc. The PI develops collaboration with Dr. Yang and Dr. Hyatt in Chemistry department

at UTC, Dr. Kim in Engineering management at UTC, Dr. Nawaz at the ORNL and Dr. Zhao at 3M.

Students Impacted

Evan Gildernew (NMX363) is a graduate student pursuing his master's. He has been working on the development of computational modeling for the water harvesting project. He has successfully developed multiple working models. He finds interest in computational research and will pursue Ph.D. program at UTC. The carryover CEACSE grant will support his study.

Syed Tareq is a PhD student who previously worked with Dr. Sou. He decided to stay at UTC working with the PI to complete his PhD study. Part of the CEACSE grant will be used to support his PhD study as well.

Community and Broader Impacts

With the preliminary result, the PI plans to build a solar grill system which can be used for various outreach events searching prospective students at the Engineering school at UTC.

Scholarly Products

Publications:

7. High Temperature Stable Aerogel by ALD Coating (in revision)
8. Enhanced Solar Receiver Efficiency Using Superhydrophobic Cost-Effective Ambiently Dried Aerogel (in progress, 50%)

External Conferences:

Oral presentation scheduled at the Solar Energy Systems Conference, AIChE, 2021.

Presentations at UTC:

2021 ReSEARCH Dialogues and Technology Symposium

Inventions or Other Intellectual Property

Three patent applications submitted to UTRF.

1. Cheap, strong, waterproof, optically transparent, thermally insulating retrofit

2. Novel Silica Precursor to Synthesize Ambiently Dried Transparent Aerogel

3. Novel Air Burning Method to Synthesize Transparent Insulator

Research Outreach & Collaboration

The PI develops collaboration with Dr. Yang and Dr. Hyatt in Chemistry department at UTC, Dr. Kim in Engineering management at UTC, Dr. Nawaz at the ORNL and Dr. Zhao at 3M.

EXTERNAL FUNDING

Proposal Submissions

Please list all sponsored program proposals submitted during the reporting period related to this or previous CEACSE awards.

Proposal name	PI or co-PI	External?	Amount requested	Cayuse #
NSF-ERI	PI	Yes	199980	21-4830
ENV-SMART	Co-PI	Yes	443405	21-4466
NSF_MRI	Co-PI	Yes	392000	21-2750
TVA	PI	Yes	150000	21-1225
Ruth S. Holmberg	PI	No	5000	

Contracts/Awards Received

Nothing available yet.

Sponsored Program Capacity Building Activities

Nothing available yet.

WHAT'S NEXT FOR THIS RESEARCH?

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

CAREER is the first target. The PI plans to build a research program that lasts more than 5 years working on the most important problem in the aerogel community.

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

Another major research focus of the PI is aerogel for water harvesting and energy efficient building applications. Transparent insulator, aerogel, can promote both research areas.

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 challenge the PI has been facing is limited researcher power. The PI plans to hire two PhD students for the upcoming year, hoping that it will improve research power. In addition, the PI plan to hire more undergraduate researchers via URaCE URTOPS Program.

FINANCIAL ACCOUNTING

N.A.

CEACSE Program – Final Report on Research Results

The Tasks and Timeline with Milestones/Deliverables

The proposed tasks and timelines are shown below for the 12-month project.

Description \ Month	1	2	3	4	5	6	7	8	9	10	11	12
Finalizing synthetic method of OTTI aerogel (10x10cm2)												
Optimizing chemical recipes for ambient dried aerogel												
Optical & thermal modling via RTE and Mie theory												
Mechanical modeling via molecular dynamics												
Builing solar collector assembly & lab testing												
Solar process heat generator design & modeling												
Constructing the solar process heat generator assembly												
Integrating PCM thermal storage in the heating loop												
Outdoor experiments with the final prototype												
Finalizing commercialization plan and form partnerships												

Research Results

1. Finalizing synthetic method of OTTI aerogel

As shown in Figure 1a, we demonstrated transparent OTTI aerogel with ~ 12 cm diameter. In our lab, we have optimized the silica aerogel fabrication recipe and processing conditions to achieve pore sizes of 2-50 nm. Carefully tailoring the nanostructure of our aerogel samples has allowed us to achieve solar-weighted transmittance greater than 96% for a 3 mm thick sample (Figures 1b) that is the highest transmittance report in the literature. As the gelation reaction (hydrolysis and condensation reactions) is exothermic reaction, the amount of catalyst should be precisely controlled for the scale-up.

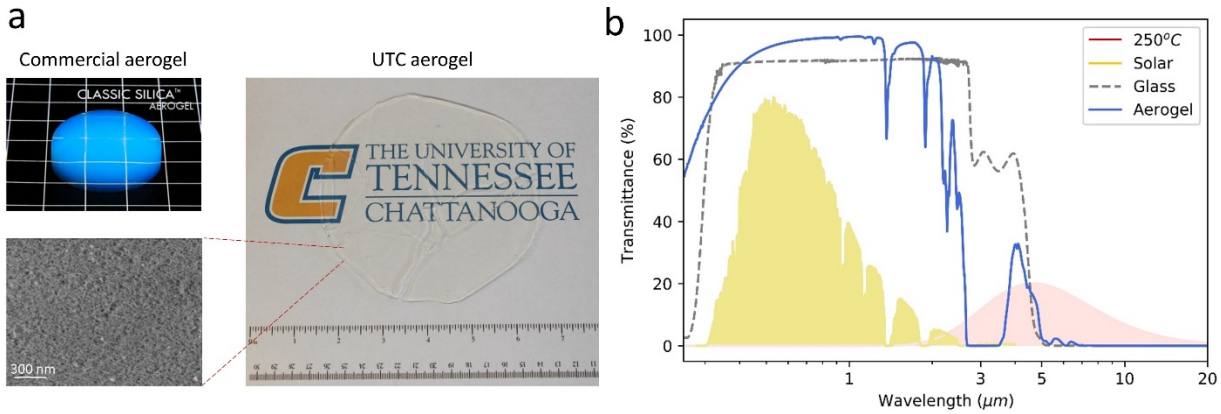


Figure 3: (a-left top) Image of commercially available silica aerogel. (a-right) Image of a 200 mm diameter monolithic silica aerogel sample fabricated in our lab. (c) Measured hemispherical transmittance of the aerogel sample (blue), showing high transparency in the solar spectrum (yellow-filled) and significant suppression of blackbody radiation (red-filled) at the target operating temperature

2. Optimizing chemical recipes for ambiently-dried aerogel

Furthermore, we have reinforced OTTI aerogels via optimizing cross-linked polymers in the aerogels. Improved mechanical properties result in ambient-pressure dried aerogels, which can greatly reduce the aerogel production cost by an order of magnitude. Figure 2a shows a reinforced ambiently-dried OTTI aerogel. It is superhydrophobic as shown in Figure 2b. Figure 2c show the transmittance (in red line) of the ambiently-dried aerogel, 90%, that is marginally higher than the best literature transmittance of ambiently-dried aerogels.

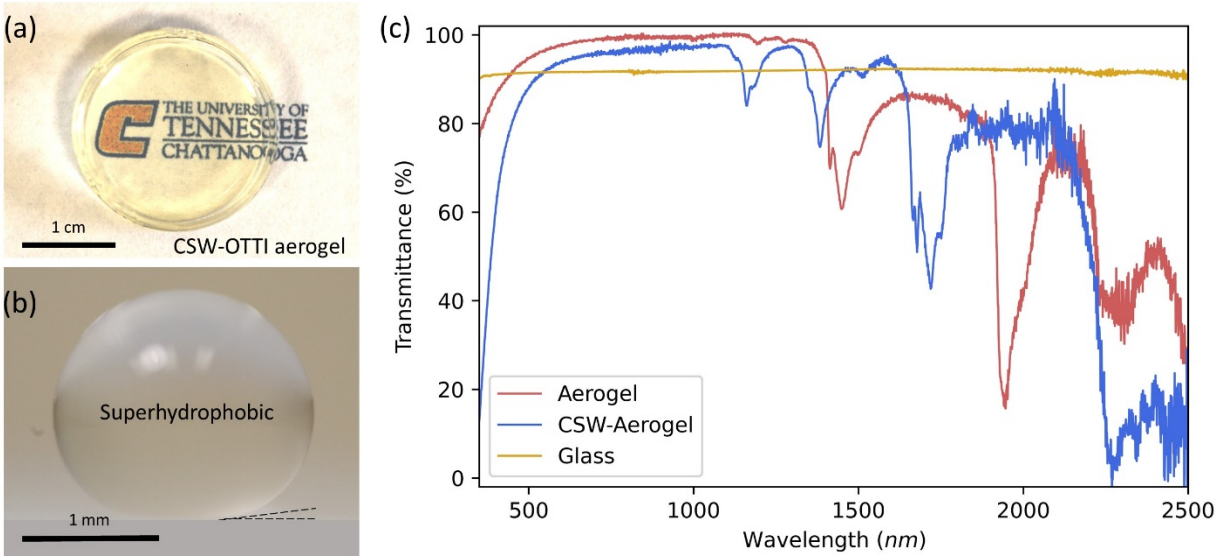


Figure 4: (a) Image of a synthesized CSW-OTTI aerogel. (b) Image of a droplet on a CSW-OTTI aerogel demonstrating its superhydrophobicity with a high contact angle (> 150°) (c) Measured hemispherical transmittance of conventional OTTI aerogel dried by CPD (red), CSW-OTTI aerogel (blue), and glass (yellow). CSW-OTTI aerogels show high transparency in the solar spectrum which is higher than the highest reported in the literature.

2. Optical and thermal modeling via RTE and Mie theory

To perform the proposed thermal modeling solving RTE equation with energy balance equation, specific extinction coefficient of the samples is required. Figure 3a shows transmittance of the samples in IR band by using FTIR. The extinction coefficient and specific extinction coefficients are deduced from the FTIR results, as shown in Figure 3b and 3c with measured sample density. Lastly, the effective emittance of the samples is calculated as shown in Figure 3d. Carbon components in ambiently dried aerogel demonstrated lower effective emittance.

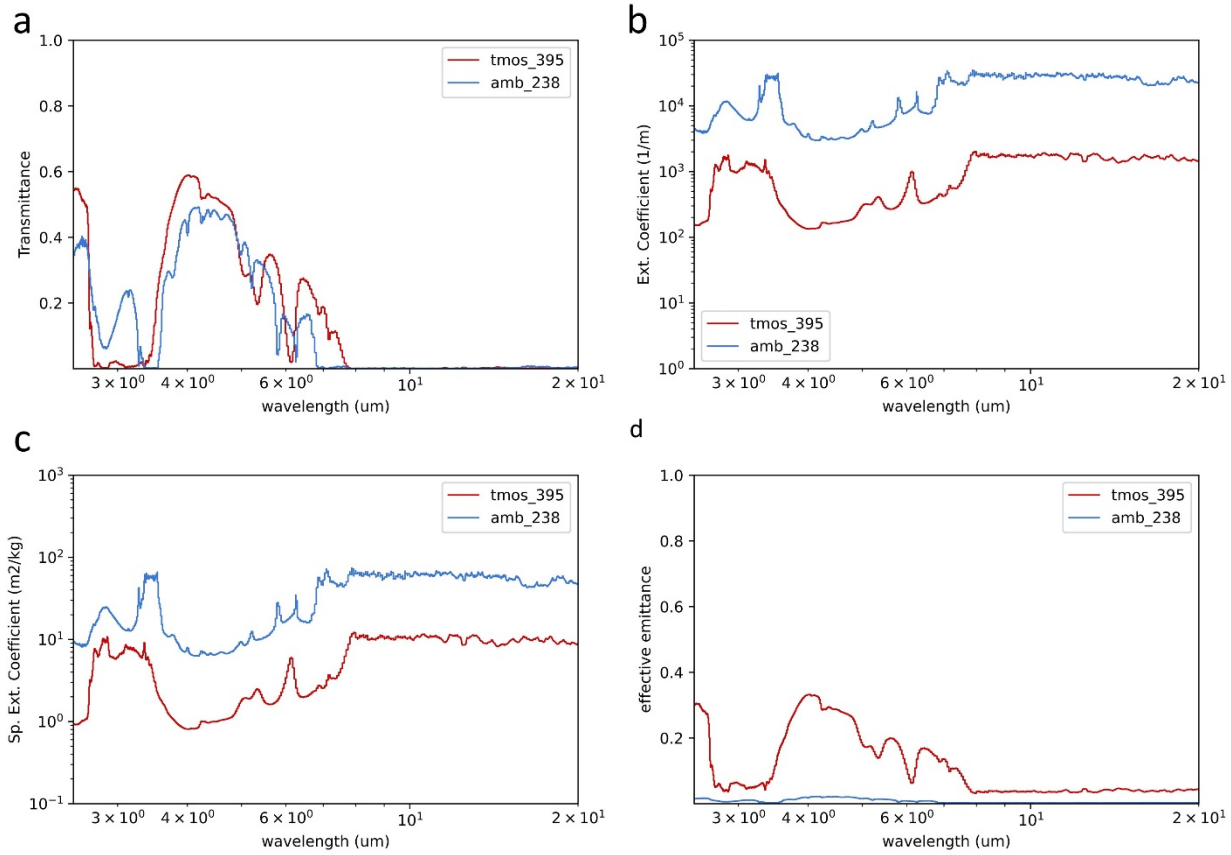


Figure 5: (a) FTIR transmittance of silica aerogel and ambiently-dried aerogel. (b) extinction coefficient and (c) specific extinction coefficient of silica aerogel and ambiently-dried aerogel (d) effective emittance of silica aerogel and ambiently-dried aerogel.

2. Building a lab-scale solar collector

As shown in Figure 4, we have built a lab-scale solar thermal collector, which will be used for outdoor testings.

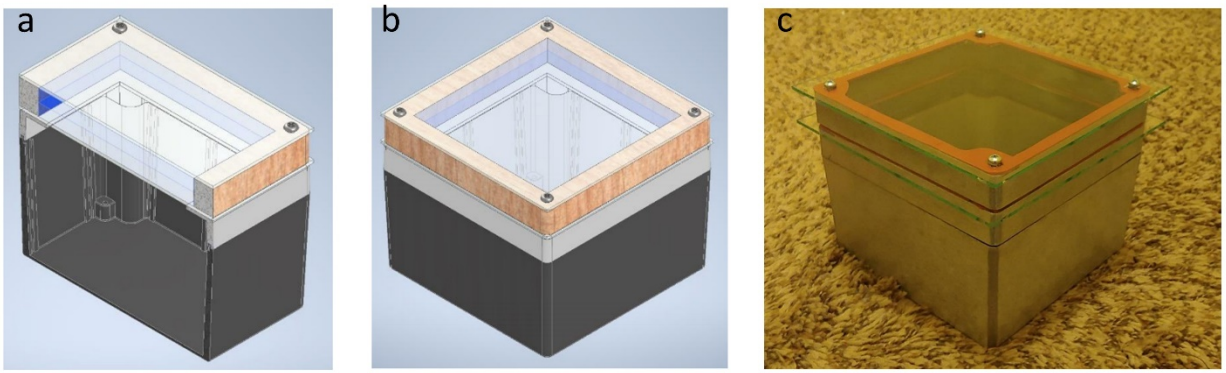


Figure 4: (a) and (b) CAD drawings of solar grill system (c) an image of the built solar grill system before the addition of transparent aerogel

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Sungwoo Yang, Lead PI

Co-PI(s): NA
Other Personnel: NA

Project Title: “Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss”

Date Submitted: 08/30/2023

Award Start – End Date: July 1, 2022 – June 30, 2023

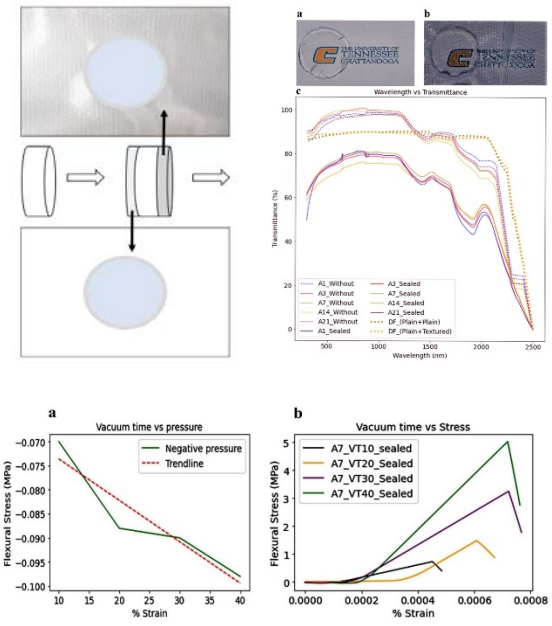
Non-Technical Summary:

The major objectives include (1) developing novel functionalized silanes as silica precursor and chemical recipe to synthesize ambiently dried CS-OTTI aerogel with record high transmittance, (2) CS-OTTI aerogel retrofits for single-pane windows with suitable scalability and machinability, (3) prototype development with computational modeling analysis. While we are still in progress of developing novel functionalized silanes, we have demonstrated vacuum sealed aerogel that can be retrofits for single-pane windows with suitable scalability. A PhD student successfully defended his PhD study based on this research. A peer-reviewed journal paper is submitted and in review. Upon completing the proposed project, the PI plan to use an energy-efficient window using aerogel for Solar Decathlon project ($100k) that was funded by the Government of California to alleviate recent climate change issue. The PI plans to request carry-over the funding until the end of 2023 to support his PhD student to continue the proposed research, but the request was denied. However, the PI plans to continue the proposed research targeting external funding.

PROJECT TITLE: “Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss”

Technology Area of Interest: Energy

TECHNICAL APPROACH	OUTCOMES
(1) developing novel functionalized silanes as silica precursor and chemical recipe to synthesize ambiently dried CS-OTTI aerogel with record high transmittance, (2) CS-OTTI aerogel retrofits for single-pane windows with suitable scalability and machinability, (3) prototype development with computational modeling analysis.	Demonstrated vacuum sealed aerogel that can be retrofit for single-pane windows with suitable scalability resulting in (1) a PhD defense, (2) a journal publication in review, (3) external funding, $100k. To continue the proposed research, carry-over requested to support a PhD student, but not approved.

RESULTS	OTHER INFO
	**Budget and Schedule** Total Budget: $99,996.00 Actual Used: $69,851.47 Balance: $30,144.53 **Deliverables** • A final report • A journal publication (Construction and building materials, Elsevier, in review) • An external funding, OCSD project ($100k) **Organization Information** *Sungwoo-Yang@utc.edu*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
developing novel functionalized silanes as silica precursor and chemical recipe to synthesize ambiently dried CS-OTTI aerogel with record high transmittance	In progress
CS-OTTI aerogel retrofits for single-pane windows with suitable scalability and machinability	Demonstrated vacuum sealed aerogel that can be retrofits for single-pane windows with suitable scalability
prototype development with computational modeling analysis	Studied computational modeling analysis

Challenges & Strategies Used to Address / Overcome:

The biggest challenge was lack of research equipment and manpower at UTC. The PI has been working closely with the Chemistry department at UTC to resolve the challenge. A PhD student is the crucial component to move this project going forward. As developing novel functionalized silanes went slower than expected, the PI requested carry-over funding, that was not approved. Yet, the development is still in progress. 1-year might not be enough to generate meaningful research results. Multiple years funding will be an efficient approach.

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

Stated in the above question.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

CEACSE grants helped my career to set up PI's laboratory and to support PI's graduate students in past years. As a result, the PI successfully received tenure at UTC, published multiple peer-reviewed journal papers and external fundings. Below is the summary.

(a) List of fundings received related with CEACSE grants

Year	Proposal	PI/Co-PI	Amount
2022	Government of California, OCSD 2023	PI	$100,000

2021	CEACSE_FY2023	PI	$99,765
2021	Brach Technology_FY2022	PI	$4,950
2021	Ruth Holmberg grant	PI	$5,000

(b) List of journal papers published related with CEACSE grants

Year	Journals	Authorship
2022	Materials	Corresponding
2022	Journal of Chemical Information and Modeling	Corresponding
2022	Catalysts	Corresponding
2023	Journal of Green Building	Corresponding

Students Impacted

- A PhD student successfully defended his PhD study
- UTC Solar Decathlon student club was created where numerous UTC students gain benefits by hand-on experiences on renewable energy research and building technologies

Community and Broader Impacts

The buildings sector constitutes about 76% of electricity use and 40% of all U.S. primary energy use and associated greenhouse gas (GHG) emissions. Windows are particularly important for the building sector as windows are responsible for 2.15 quadrillion Btu (Quads) of heating energy consumption and 1.48 Quads of cooling energy consumption annually.1 While advanced window technologies could offer energy savings potentials of up to 3.9 Quads, affordable manufacture remain a significant barrier to widespread implementation. Single-pane windows are ubiquitous and constitute the most energy inefficient component of our building envelopes. Existing solutions include replacement with insulated glass units or air-filled double-pane windows which are quite expensive and are often incompatible with existing frames. Alternate low-cost solutions primarily rely on retrofitted low-e coatings that are capable of reducing the radiative heat loss from the indoors, but are susceptible to condensation during winters, which renders them ineffective and undesirable. The development of a cheap, strong, optically transparent, thermally insulating (CS-OTTI) retrofit for a single-pane window is achievable, deliverable, and capable of dramatically reducing energy consumption in buildings nationwide, particularly during winter.

Scholarly Products

Publications:

- S. Tareq, M. Colson, E. Gildernew, S. Friedman, and S. Yang, Enhancing Mechanical Properties of Low Scattering Transparent Insulating Aerogel through Vacuum Packaging and Visualize Insulant Performance, Construction and building materials, Elsevier (in review)
- Black, N.; West A.; Yang, S.; et. al. Design a Net Zero House at 100-Year Flood Zone in a Historic District: A Case of Solar Decathlon Design Challenge Entry. Journal of Green Building 1 January 2023; 18 (1): 243–263. https://doi.org/10.3992/jgb.18.1.243
- Colson, M.; Alvarez, L.; Soto, S. M.; Joo, S. H.; Li, K.; Lupini, A.; Nawaz, K.; Fomunung, I.; Onyango, M. A.; Danquah, M. K.; Owino, J.; Yang, S. A Novel Sustainable Process for Multilayer Graphene Synthesis Using CO2 from Ambient Air. Materials 2022, 15 (17), 5894. https://doi.org/10.3390/ma15175894
- Gildernew, E.; Yang, S., Finite Element Modeling of Atmospheric Water Extraction by way of Highly Porous Adsorbents: a roadmap for solver construction with model factor sensitivity screening, Journal of Chemical Information and Modeling, 2022 August. https://doi.org/10.1021/acs.jcim.2c00683
- Gildernew, E.; Tareq, S.; Yang, S. Three-Dimensional Graphene with Preserved Channeling as a Binder Additive for Zeolite 13X for Enhanced Thermal Conductivity, Vapor Transport, and Vapor Adsorption Loading Kinetics, Catalysts 2022, 12(3), 292; https://doi.org/10.3390/catal12030292

External Conferences:

- NA

Presentations at UTC:

- ReSEARCH Dialogues and Tech Symposium

Inventions or Other Intellectual Property

UTRF disclosure (UTRF # 21164-02) submitted.

Research Outreach & Collaboration

Research collaboration with Dr. Kashif Nawaz, Section Head - Building Technologies Research; Group Leader - Multifunctional Equipment Integration at Oak Ridge National Laboratory

EXTERNAL FUNDING

Proposal Submissions

2023	FLY competition

2023	EnergyTech UP 2023
2022	NSF-MRI-FY2023
2022	NSF-ERI-FY2023
2022	NSF REU-iGREEN
2022	Search
2022	OCSD
2022	NSF S-STEM
2022	DOE-SIPS
2022	EREF
2022	NSF-MRI-FY2022

Contracts/Awards Received

2023	FLY competition ($22k)
2022	OCSD ($100k)

Sponsored Program Capacity Building Activities

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 plans to continue conducting research on the proposed research. But the lack of graduate students is expected to be the biggest challenge.

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

Design and build an energy-efficient house

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

I believe it will make a send to fund at least two years. One year is too short.

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

Stated above.

FINANCIAL ACCOUNTING

Stated above.

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Smith, Morgan F., Lead PI

Co-PI(s): Boris Belinsky; Chris Cox
Other Personnel: Gage Plott, Carla Adamson, Tyler Mullins, Maddie Shaw

Project Title: "Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites"

Date Submitted: October 2022

Award Start – End Date: July 1, 2022 – June 30, 2023

Non-Technical Summary:

Our objective was to test, through numerical modeling, simulations, and controlled experiments, a method of detecting anthropogenic lithic material (stone tools) remotely with a sub-bottom profiler (SBP) as a means of identifying underwater archaeological sites rapidly and non-invasively. We used this funding to work toward the application of a computer code for modelling and simulating this phenomenon, with the eventual goal being to move toward machine learning and automation of this methodology. This project is necessary because the reliability of this method in the field is unknown, and further tests were needed to control environmental variables which cannot be mitigated in the field (water temperature, density, turbidity, etc.). Our project fulfills CEACSE's primary funding goals, as it concerns modelling, simulation and machine learning, will result in high-impact peer-reviewed publications and, if successful, will seed future long-term funding from external sources.

This project had several notable outcomes, including:

- Successful construction of computer code from scratch in FEniCS. The code building was a labor-intensive effort and was spearheaded by graduate students at UTC. With the code built, iterative experiments can be conducted beyond the timeframe of the grant which can be used for further experimentation.
- Independent, successful replication of the initial modelling experiment that first proposed this methodology, with some minor variations.
- Successful laboratory trials at the U.S. Navy Transducer Evaluation Center (TRANSDEC), an anechoic chamber in San Diego, CA.
- Successful controlled field trials in three separate geographic areas over renowned submerged archaeological sites in Baja California Sur, Mexico; Southampton, England; and Alpena, Michigan.
- Wages for four students who assisted in this research, two graduate and two undergraduate.
- This research will form the cornerstone of two PhD dissertations in the mathematics department at UTC and one in Mexico. It also served as the subject of a graduate student's first conference presentation and an undergraduate student's first poster presentation at UTC's Research Dialogues Conference this spring.

- This research will seed at least one external grant application and two peer-reviewed works in the 2023-2024 academic year.
- Acquisition of cutting-edge SONAR equipment to support ongoing research and student training at UTC. This equipment firmly places UTC among the most well-outfitted underwater archaeological academic programs in the country.
- This research both supported the mission of the SimCenter and advanced it in new directions. Specifically, the research focus area supported by this work was energy and the environment. Our research could expedite offshore capital development and renewable energy projects without sacrificing impact to cultural resources, lessening impact to the human and natural environment. As these projects grow, UTC is well-positioned to exploit a niche in offshore renewable energy with this fundamental research (Figure 1). Our work advanced the SimCenter into a novel but growing area of applied mathematics and geophysics, as well as smarter, next-generation methods for cultural heritage preservation through numerical modelling and computer simulations.

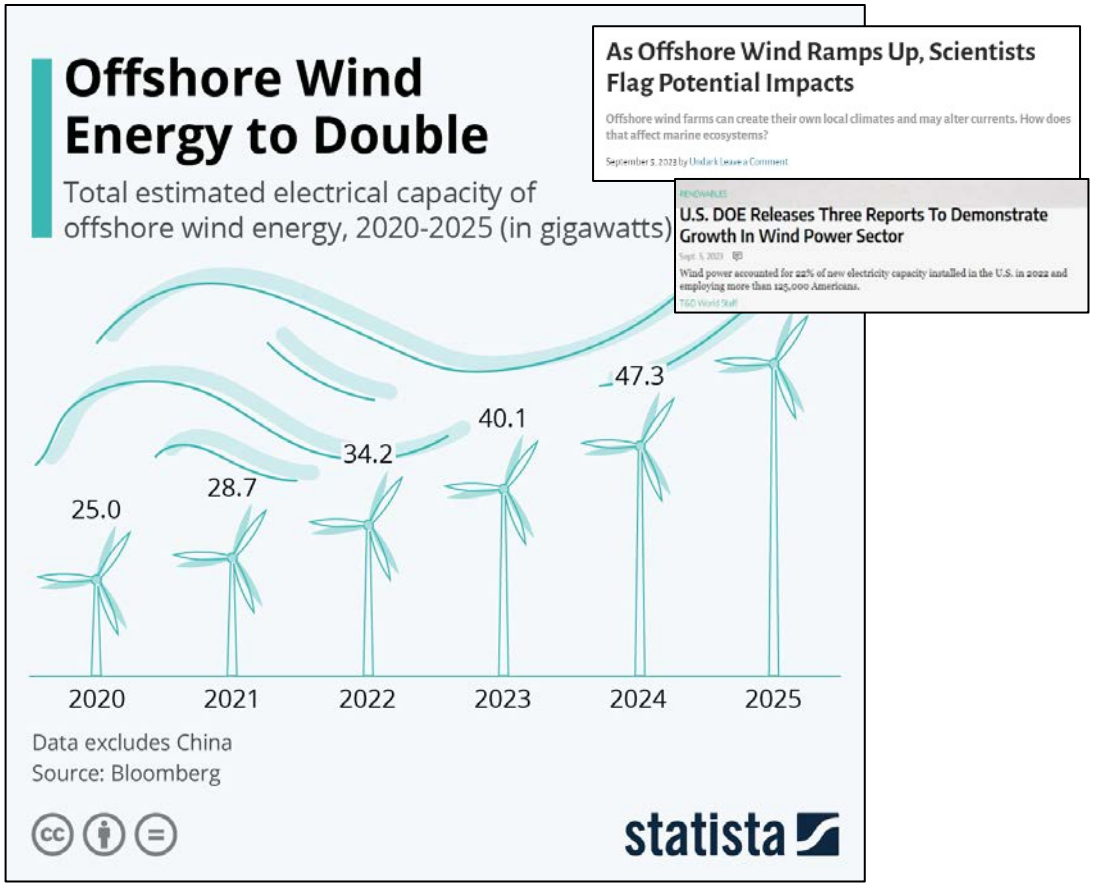


Figure 1. Offshore wind is expected to double by 2025 but is still somewhat a “wild-west” in terms of regulations and standards within the industry. Offshore resource exploitation in general is accelerating and with it, so are financial and employment opportunities.

TECHNICAL APPROACH	OUTCOMES
- Replicate the foundational modelling study demonstrating this phenomenon (Hermand et al. 2011). - Develop a code in FEniCS to conduct iterative experiments. - Conduct field trials to collect geophysical signatures of known sites in myriad environments. - Acquire instrumentation to build capacity at UTC for future testing.	- Construction of code allowing for replication of this crucial study and further modelling experiments. - Acquisition of geophysical signatures from 8 submerged prehistoric sites in North America and Europe. - Exposure of UTC's cutting-edge research to R1 schools in the US and abroad. - Acquisition of sub-bottom SONAR systems at UTC to enhance research capacity locally and train students on next-generation technology. - Training of undergraduate and graduate students in archaeology and numerical modelling. - This project is a component of two doctoral dissertations at UTC, one abroad, and two research posters by undergraduate students. - This research is being prepared for publication in two scholarly journals. - This research will serve as the foundation of an external grant application.

RESULTS	OTHER INFO
See below, Figures 2-9 and subsequent paragraphs.	**Budget and Schedule** Total Budget: $ 99,938.00 Actual Used: $ 98,337.63 Balance: $ 0.00 Salary, Smith $ 19,015.25 Salary, Belinsky $ 7,911.00 Salary, Plott $ 1,900.00 Salary, Undergraduates $ 1,523.50 Benefits from Salary $ 4,620.23 Travel $ 11,539.94 Shipping $ 15,045.93 Materials and Supplies $ 3,612.07 Rentals $ 11,913.45 Contracts $ 2,398.90 Motor Vehicle Ops $ 1,357.36 Equipment $ 17,500.00 Total period of performance was 12 months. Task 1: Months 1-3 - Organize team. - Define action items for objectives. - Literature review and background research. Task 2: Months 3-6 - Formulate code. - Run first simulations. - Present preliminary data at international conference. Task 3: Months 6-12 - Refine code and conduct simulations. - Collect field geophysical data from known sites and disseminate technical approach to practitioners. - Acquire geophysical and acoustic equipment to continue research at UTC post-grant. Task 4: Months 12 - Write final report. - Prepare publication of results. - Begin preparation for NSF proposal.

Figure 2. SONAR survey vessel in preparation for work in Baja California Sur, Mexico.

Figure 3. SONAR survey underway in Baja California Sur, Mexico.

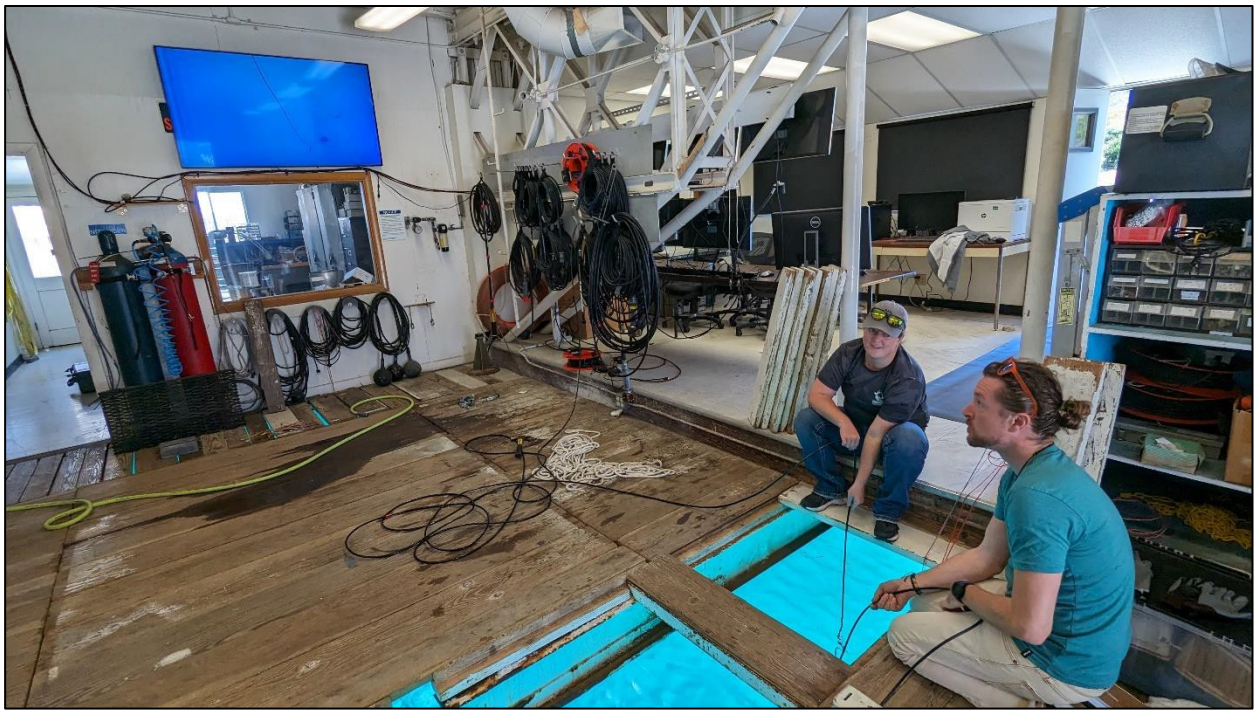


Figure 4. SONAR testing underwater at the US Navy Transducer Evaluation Center, San Diego, CA.

Figure 5. SONAR testing underwater at the US Navy Transducer Evaluation Center, San Diego, CA.

Figure 6. SONAR testing underwater at the US Navy Transducer Evaluation Center, San Diego, CA

Figure 7. SONAR testing underwater at the Bouldnor Cliff site in the Solent, Southampton, UK.

Figure 8. SONAR testing underway with UTC students on the Tennessee River, Chattanooga, USA.

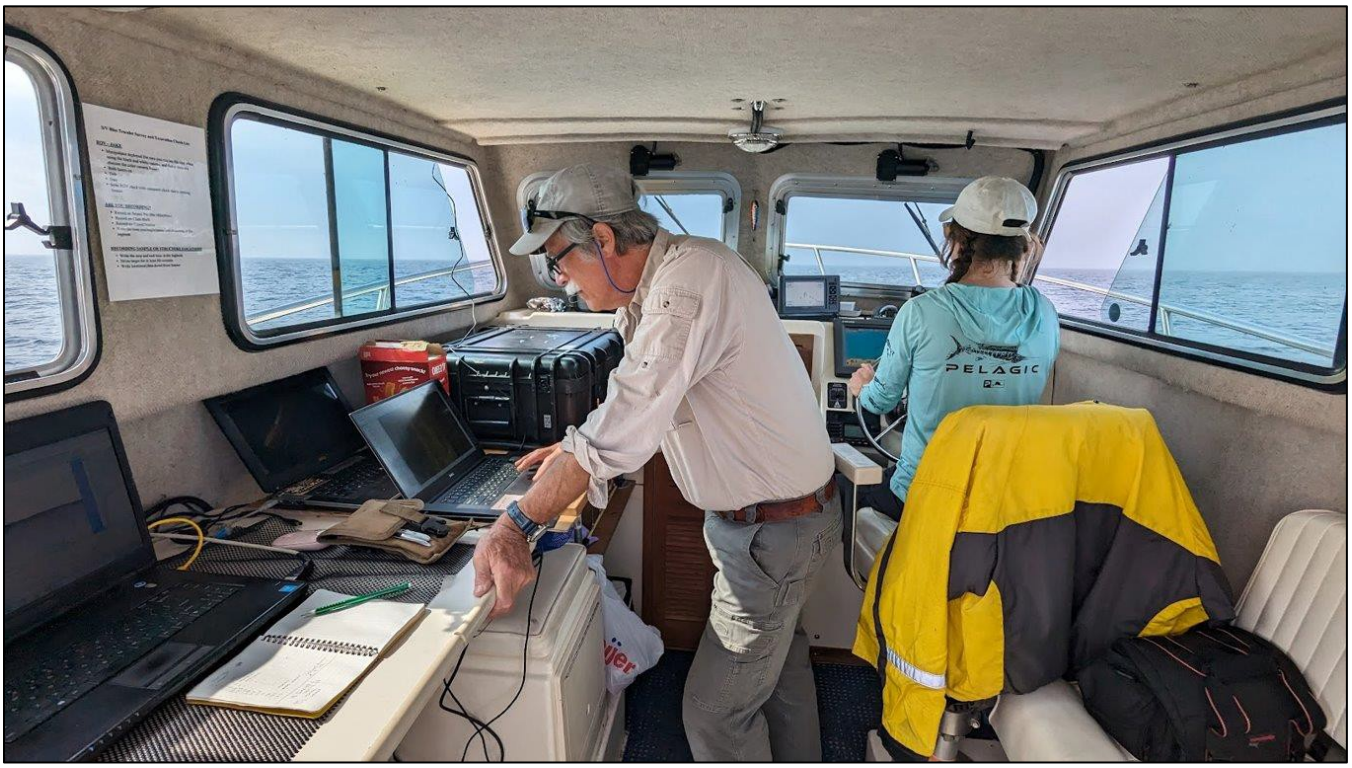


Figure 9. SONAR testing underway with colleagues at the University of Michigan on Lake Huron, USA.

ACCOMPLISHMENTS & OUTCOMES

Project Overview

In 2011, a potentially groundbreaking paper was published. It received little fanfare, perhaps due in part to its niche but impactful claims that acoustic (pressure) waves could be used to remotely identify archaeological sites underwater.

Context for this paper is important. Due to rising sea-levels worldwide, archaeological sites which were once on dry land are now underwater (Figure 10). Globally, this now inundated landmass equates to roughly the size of modern-day South America. This is relevant because the continental shelves of the world have recently been targeted as areas for extensive capital development, including offshore wind and renewable energy, sand and minerals mining, as well as ever present oil and gas exploration. In the United States, offshore resource exploitation within the US Exclusive Economic Zone is subject to federal law that requires archaeological (among other) surveys be conducted before development occurs. However, no method exists for identifying indigenous sites on our continental shelves. We know that the earliest people to enter the Americas arrived before 16,000 years ago, and that they occupied now submerged lands. However, finding these sites is extremely difficult, as they represent hunter-gatherer groups who are typically light on the land and sea-level rise has obscured

obvious indicators of site presence. Conversely, historic resources, such as shipwrecks, are readily found by a number of methods, as they contain metal and typically stick above the seafloor. As indigenous sites are difficult to locate, they are being destroyed at an unknown rate while shipwrecks are preserved, creating an equity crisis: more indigenous patrimony exists on submerged lands than European shipwrecks, yet recorded shipwrecks outnumber indigenous sites by several orders of magnitude. A solution to this problem in the US would have immediate global impacts.

If sound waves within a certain frequency and amplitude can identify stone tools, then multiple problems can be solved simultaneously. First, underwater cultural heritage can be more adequately preserved worldwide with an emphasis on traditionally underrepresented groups, a priority under the current UNESCO (United Nations Educational, Scientific, and Cultural Organization) charter. Second, we can accelerate offshore capital development to address clean-energy and climate-change related problems without sacrificing cultural heritage documentation and protection. Third, archaeological sites often contain datasets relevant to the fields of genetics, biology, geology, climatology, and paleontology. Thus, this method could result in a cascade of new discoveries and novel research questions.

Yet, extraordinary claims require extraordinary evidence. Replication studies are paramount to solid science yet are infrequently conducted. The PI of this project, upon seeing this paper, attempted field replication of the study with success, which attracted funding from the National Science Foundation, and affirmed the fundamental premise. Off the shelf geophysical instruments can, under certain circumstances, be used to identify underwater indigenous sites. However, much further research is needed into why this method works. To that end, we undertook an extensive effort to develop code to run simulations on this phenomenon, conduct limited laboratory and field trials, and engage students in the process.

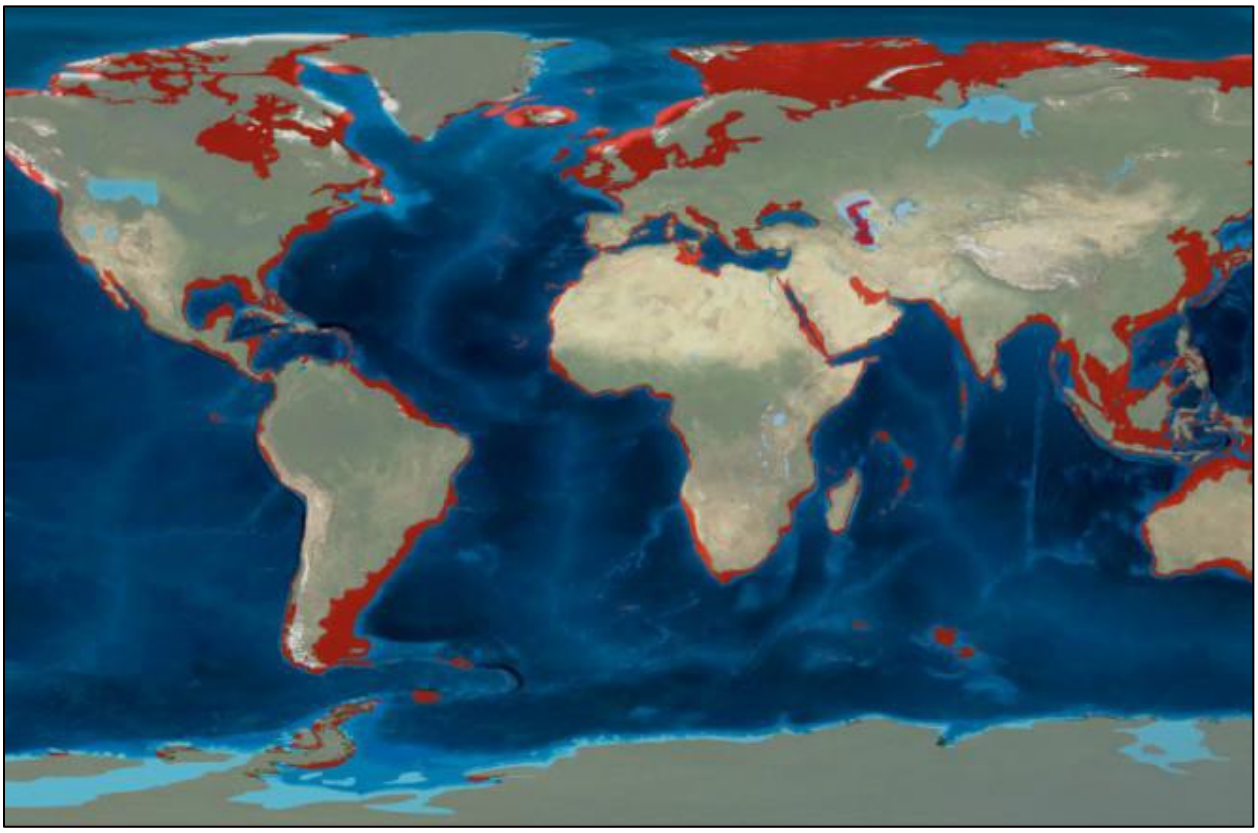


Figure 10. Global map showing land that was once exposed (in red) but is now submerged due to rising sea levels. Image Credit: Deep Time Maps/Alison Mackey/Discover.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Adapt the previously used code for numerical modelling of acoustic phenomena.	• Code proposed could not be adapted. • Instead, an entirely new code was written from scratch in a newer, more powerful coding package which, although much more time-intensive, was a remarkable achievement. • The code is now able to be used for continuing experimentation at UTC, able to support student and faculty research into this matter beyond the life of the grant.
Develop numerical model and conduct simulations of acoustic wave interactions. Replicate the original study and conduct novel experiments. Conduct controlled lab and field experiments.	• This was achieved, and a replicative study of the original proposed paper was successful, with a few aberrations (described below). • Controlled lab trials were conducted at the US Navy Transducer Evaluation Center, San Diego, CA. • Controlled field trials were conducted in the Tennessee River (USA), Gulf of California (MX), Lake Huron (USA), and the Solent (UK). • Further iterative studies were planned, but not all were achieved. However, now that the code is complete, this work may continue and will be completed this Fall.
Prepare final report and draft manuscript for peer review.	• Report herein. • Two publications planned, one targeted for Journal of Archaeological Science and the other for Journal of Applied Mathematics.

Challenges & Strategies Used to Address / Overcome:

The primary challenges for this research were personal and personnel issues. The unanticipated departure of one of the original primary investigators, Abi Arabshahi, in August at the onset of the project left the modelling side of the grant largely vacant. However, with help from Dr. Skjellum, we re-organized with an excellent team which brought in Dr. Christopher Cox and PhD student Gage Plott in Abi's stead. In December, my wife nearly passed away from severe surgical complications, necessitating an extended pause in all grant and work activities. Her medical issues remained through the early spring and one of the PhD students, Gage Plott, needed to step away from the program for personal reasons suddenly in April.

Fortunately, my wife's health fully returned in the spring and another PhD student, Carla Adamson, stepped in over the summer to help us cross the finish line.

We did also face a problem in that the original coding package, SPECFEM, was difficult to obtain, written in an outdated format, and contained numerous errors, prohibiting its application for this project. Thus, we were forced to pivot to developing our own code from scratch in a new package, FEniCS.

Fundamentally, our stated hypotheses to test were:

1) Low-frequency sound waves create structural resonance in stone tools which can be observed within the range of SBP equipment (4-24kHz).

2) Low-frequency sound waves do not create structural resonance in other materials (ceramics, bone, shell, etc.) within the range of SBP equipment (4-24kHz). That is to say, only stone tools resonate within this spectrum and the signatures seen in SBP data are exclusively those produced by stone tools.

Despite the aforementioned problems, we managed to achieve nearly all of our original objectives as outlined in the proposal. We had initially proposed the following objectives, where objectives 1, 2, 3.a, and 4 are achieved and Objectives 3.b-e are in progress.

1) Build a code in a finite element coding package to simulate acoustic wave interaction with stone tools.
2) Replicate the Hermand et al. 2011 study.
3) As effort and time allow, conduct the following simulations:
    a. Variability of resonant material
    b. Resonance of surface scatters
    c. Lithic density (1x1m square covered 25,50,75,100)
    d. Lithic shape
    e. Environment
4) Controlled lab and field simulations of the method.

One of two challenges for this effort was to duplicate modeling results for a problem that was not fully described in the primary reference:

> J.-P. Hermand, O. Grøn, M. Asch, Q. Ren, "Modeling flint acoustics for detection of submerged Stone Age sites". Proc. OCEANS'11 MTS/IEEE Kona Conf. (Oceans of Opportunity: International cooperation and partnership across the Pacific), Institute of Electrical and Electronics Engineers, IEEE, Sept. 2011.

For example, units are not specified for pressure, and the range of pressure values in one of the figures is from -2 x 1015 to 2 x 1015. The second challenge came with the recognition that there is a typo in the main governing equation, equation (1) in this paper:

The '2' should not be there, according to several reliable sources, including these notes from a graduate course at the University of Texas:

> http://www.ae.utexas.edu/courses/em397_shocks/Chapter_2.pdf
>
> and also:
>
> https://en.wikipedia.org/wiki/Linear_elasticity
>
> (see the time-dependent form of the equation identified as the Navier-Cauchy equation).

Furthermore, the authors do not provide information about the relationship between displacement (the solution of the equation given above) and pressure (the variable in the plots). Precise locations for the flint pieces are lacking - the authors only state "they are placed at slightly different depths in the cultural layer."

Our strategy for modeling started with a thorough literature search to confirm the correctness of the model we are using and to find other numerical results for comparison to ours. We found the following paper:

> R. T. Boumda and J. -P. Hermand, "On the acoustic detection of flint blade in soft sediment," 2013 IEEE/OES Acoustics in Underwater Geosciences Symposium, Rio de Janeiro, Brazil, 2013, pp. 1-4, doi: 10.1109/RIOAcoustics.2013.6684001.

that solved the same problem (also with a typo in the governing equation) and had a few more details, including specifying units for pressure in one of the figures.

For the numerical solution of the mathematical model, we chose to use the FEniCS finite element software platform. This is a state-of-the-art and well-supported open-source package for solving mathematical models posed in the form of partial differential equations, that uses the python programming language. The FEniCS Project was initiated in 2003 as a research collaboration between the University of Chicago and Chalmers University of Technology.

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

In general, our work failed to disprove the fundamental concepts authored by Hermand et al. in 2011. Our field trials had limited success, including a lack of noticeable resonance signatures at one of the known sites surveyed in the UK. We also had varying success in the controlled lab trial at TRANSDEC. Thus, we learned that while the modelling works, some more refinement is needed when translating this method to the field: a problem we anticipated but confirmed in this study. We also did not generate results that fully agree quantitatively with the Hermand, et al. results, though there is sufficient qualitative agreement to support the conclusion that we have a useful model. Consider the following figure from the Boumda and Hermand paper (Figure 11) that displays the simulation result for pressure at a hydrophone near the acoustic source. The three curves represent pressure when a flint blade is on the seabed, pressure when there is no flint blade, and the difference between these plots. The scale for the latter curve is different than the first two, varying from -500 to 500 (indicated on the right-hand side) rather than -5000 to 5000 that is on the left-hand side.

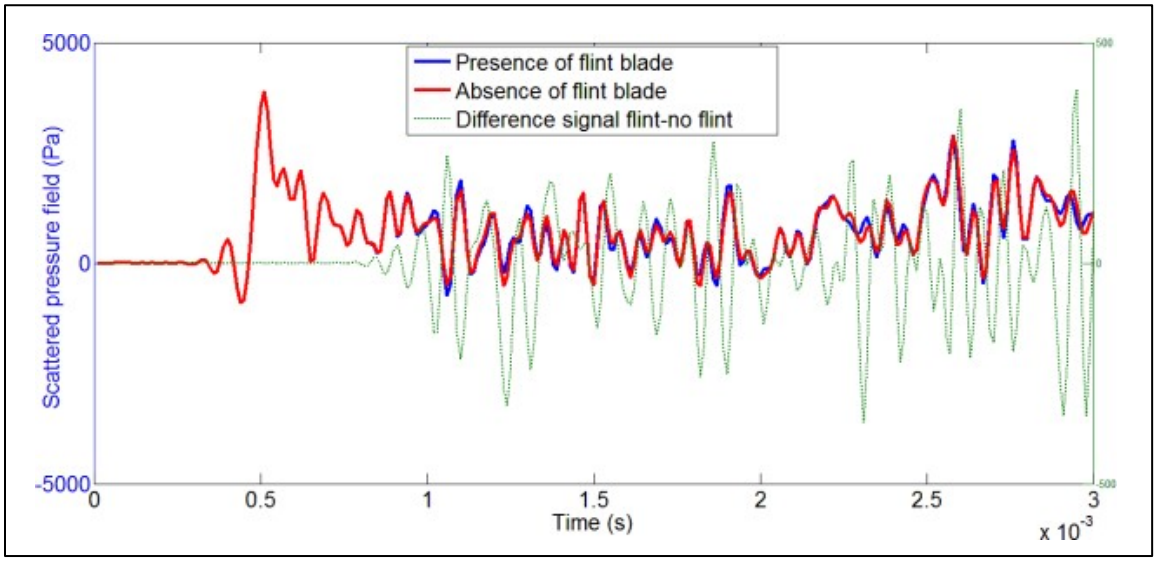


Figure 11. Result from Boumda and Hermand 2013, which we attempt to replicate in this study.

Our FEniCS result is in the figure below (Figure 12). While there is quantitative difference, we note that the trends and order of magnitude of the results are similar. For each figure (Figure 11 and 12), the nonzero difference between the no flint and flint cases begins at nearly the same time. Our scale is from -2000 to 2000 for each curve, so the magnitudes of the values are similar for a wide range of time values. We are encouraged by these results and have actionable ways forward.

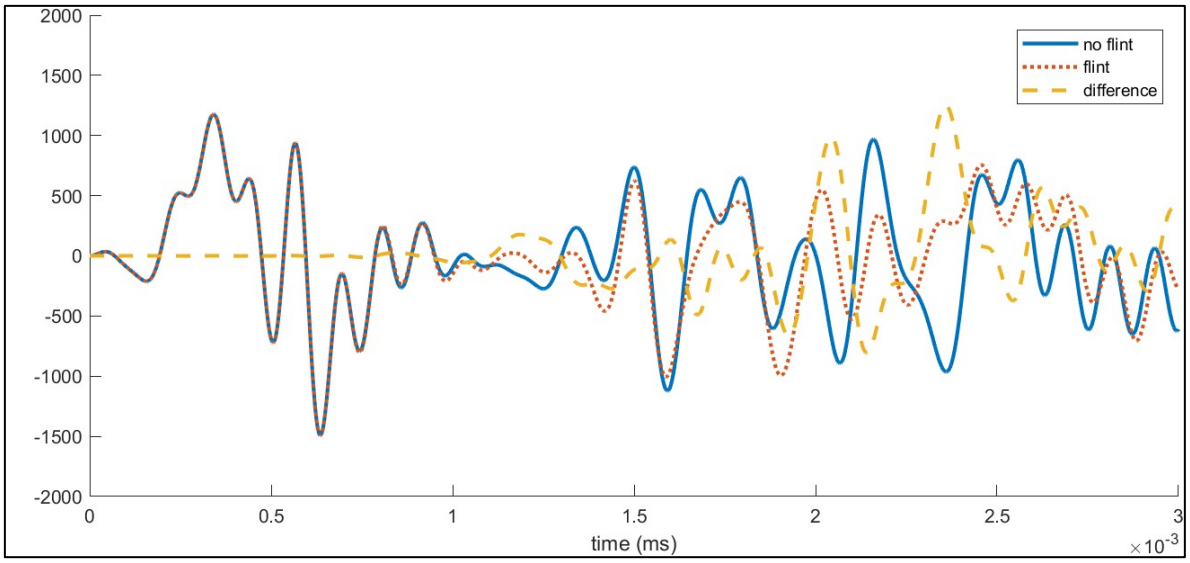


Figure 12. Result from our study, showing a difference between measurements but not a quantitative match with the above study.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

PI

This award had a measurable impact on the PI, Morgan F. Smith. This award was received prior to Dr. Smith applying for tenure and promotion to Associate Professor, and the award certainly assisted in that regard. The award also allowed Dr. Smith to increase his international profile, and that of UTC's archaeology program, with world-class institutions. National and international recognition are prerequisite to full professorship, and this award facilitated that exposure. This award also provides significant foundational studies that Dr. Smith can continue working on, serving as source material for external funding and scholarly articles for several years as this research develops. Finally, this award introduced Dr. Smith to remarkable colleagues at UTC and fostered an ongoing, multi-disciplinary working group that would not exist otherwise.

Co-PI's

This research effort is beneficial to the math faculty (Belinskiy and Cox) that have been involved as they have been introduced to an interesting application area that will likely generate a research publication in the near future. It is expected that at least one PhD dissertation will result from this work, with a likelihood of research opportunities for more students.

Students Impacted

Two math PhD students, Carla Adamson and Matthew (Gage) Plott honed programming skills and gained valuable interdisciplinary research experience. Gage developed the initial program and then for personal reasons stepped away from the PhD program (and will return in January). Gage handed the code to Carla at the beginning of the Summer and Carla implemented the flint

artifact placement in the layered media along with absorbing boundary conditions on the sides of the computational domain. The plan for Carla is to extend her work this summer into a PhD dissertation, beginning with a PhD doctoral research course with Professor Cox this Fall.

Two Anthropology undergraduate students, Tyler Mullins and Madison Shaw, acquired experience in viewing and analyzing SONAR datasets for archaeological signatures: experience typically only available to graduate students at other underwater archaeological programs.

Madison has now graduated with plans to attend graduate school for anthropology and Tyler, still in our program, gave his first research presentation on the topic at UTC's Spring Research and Arts Conference in 2023 and remains involved in this research.

Community and Broader Impacts

Overall, this project has the primary broader impact of enhancing the preservation of indigenous landscapes, a growing prerogative of native groups. Since arriving at UTC, Dr. Smith has communicated with the Tribal Historic Preservation Offices of the Muscogee (Creek) Nation and the Eastern Band of the Cherokee Indian, both of whom are eager to see more research of this kind performed in the Tennessee River. The Tennessee River serves as a useful laboratory for this work, as it is a weather-tame water body that contains hundreds of submerged indigenous sites in the immediate vicinity of Chattanooga.

This is a problem that is tailor-made for an interdisciplinary team such as Professors Smith, Belinskiy, and Cox and their students. Professor Smith sought help with developing a model similar to one described (with some incompleteness) in the literature and developed by a team whose leader has unfortunately passed away. Applied mathematicians with expertise in modeling physical systems use experiences like this to show the impact they can have and illuminate the importance and usefulness of their field.

Scholarly Products

Software:

- FEniCS code (See Addendum 1)

Publications:

- Tentative Title "Mathematical Equations for Measuring the Presence of Absence of Materials on the Seafloor." Target: Journal of Applied Mathematics. Anticipated submission by December, 2023.
- Tentative Title "Resonance and Archaeological Site Detection: Possibilities and Problems." Target: Journal of Archaeological Science. Anticipated submission by January 2024.

External Conferences:

- Symposium co-organizer and co-chair: "Re-Visualizing Submerged Landscapes." Society for Historical Archaeology, Lisbon, Portugal, 2022.
- Co-Author: "The Human-Altered Lithic Detection System (HALD) in Real-World Situations, Acoustically Mapping of Submerged Pre-contact Sites in the Gulf of Mexico." Society for Historical Archaeology, Lisbon, Portugal, 2022.

Presentations at UTC:

- "Simulation of Wave Propagation Used for the Detection of Submerged Stone Age Artifacts." Gage Plott, Christopher Cox, Boris Belinskiy, and Morgan Smith. UTC Spring Research and Arts Conference, 2023.
- Tyler Mullins. "A Cost-Effective Approach to Mapping Submerged Landscapes." UTC Spring Research and Arts Conference, 2023.

Inventions or Other Intellectual Property

Since this method has been published previously, we do not believe that we are able to hold or apply for the patent.

Research Outreach & Collaboration

As a result of this project, I have a new, ongoing working group with colleagues and graduate students in the Mathematics Department at UTC (Drs. Chris Cox and Boris Belinsky), the Geophysics Department at the University of California, San Diego (Dr. Margaret Morris), the Department of Earth and Environmental Sciences at San Diego State University (Dr. Jillian Maloney) the Anthropology Department at the University of Michigan (Dr. John O'Shea), the Anthropology Department at the University of Wisconsin – Milwaukee (Dr. Ashley Lemke), the Department of Anthropology at George Washington University (Dr. David Thulman), the Department of Marine Sciences at the Centro de Interdisciplinario de Ciencias Marinas (Baja California Sur, Mexico, Dr. Enrique Nava), and the Maritime Archaeology Trust (Southampton, United Kingdom, Dr. Garry Momber and Mr. Brandon Mason).

Events hosted through this award included monthly meetings of math and anthropology faculty on campus, alternating between our departments where we showcased various software and hardware related to this research. We also hosted Dr. David Thulman on campus in November, 2022, and Dr. Margaret Morris via Zoom in March, 2023. Both visitors were hosted in the Department of Mathematics conference room.

EXTERNAL FUNDING

Proposal Submissions

- Three external proposals were submitted that relate directly to this proposal.
    - "Cultural and Technological Responses to The Early Holocene in the Great Lakes." The University of Michigan will lead this award, submitted to the NSF Archaeology program. This proposal, submitted in August 2023, would subaward UTC $16,428, and is being decided.
    - "Reevaluating BOEM's Guidelines for Identifying Submerged Pre-Contact Archaeological Sites in the Gulf of Mexico." Florida State University will lead this award, submitted to the Bureau of Ocean Energy Management. This proposal, submitted in August 2023, would sub-award UTC $99,996, and is being decided.
    - "Using the Tennessee River Near Chattanooga to Revolutionize Methodology and Education in Submerged Precontact Archaeology." I submitted this first to the CAREER program at NSF and then to the archaeology program with UTC as

lead. This proposal, last submitted in February 2023 for $343,121, was not funded.

Contracts/Awards Received

- No awards have been received (yet) as a result of this research.

Sponsored Program Capacity Building Activities

This award has built capacity for future research in three primary arenas:

1) Grant funds were used to secure cutting-edge SONAR equipment, including an Innomar SES Compact Parametric Sub-Bottom profiler and an Edgetech 3200 chirp sub-bottom profiler. To my knowledge, UTC is one of perhaps a handful of academic institutions in the country to possess the Innomar system and is certainly the only Anthropology program with one. Having these instruments in our possession not only makes us attractive additions to larger projects (this is already the case with the Florida State University and University of Michigan contracts), but it will make us more competitive for research grants and enhance the skills of our graduates, making them exceptionally qualified for careers in SONAR survey.
2) Grant funds were also used to develop a code from scratch which can be used to rapidly test pressure waves interactions with stone tools in many environments and with many variables. This is crucial, as common critiques of the method, including the effect of environmental variables like salinity, burial substrate, lithic size and shape, etc., can now be tested.
3) Grant funds were also used to build a small acoustic experimentation set-up at UTC, which can be used to move our modelling efforts one step forward into a controlled laboratory environment. Combined with further modelling experiments, these efforts can lay the foundation for further external funding and publication of this exciting research.

WHAT'S NEXT FOR THIS RESEARCH?

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

There are several opportunities for further research.

1) Implementing boundary conditions on the lateral sides of the computational domain that simulate an infinite region is challenging. We are using a technique called "Perfectly Matched Layers." The video created from our code, at

https://utchattanooga.instructuremedia.com/embed/01846b45-866f-4fe6-9a94-3b17e2b325d7

shows the pressure wave emanating from a source and reflecting back much more from the lower and upper boundaries than from the side, as it should. There is some fine-tuning that still needs to be done. The parameters for the model come from the Hermand paper.

2) A longer-term extension of our study is to explore the possibility of identifying the shapes of the artifacts in the cultural layer. A possible plan for this study is:

- Approximate a collection of flint objects on or in the seabed, each as a polygon.
- Use finite element analysis to find the first several eigenvalues of these polygons.

- Use these eigenvalues to find the eigenfrequencies of the elastic plates in the form of the corresponding polygons. Remove eigenfrequencies that do not belong to the interval of frequencies emitted by the experimental device.
- Find the resonance frequency from the experimental set closest to this eigenfrequency.
- Vary the corresponding polygon to minimize the difference between these two frequencies. This “optimal” polygon will represent the best form of the object on the sea floor we may identify with the help of experimental data.
- Proceed similarly with other resonance frequencies.

The goal is to either find a new form of the object or get an object of the same form. This approach could be used, potentially, to build a large dataset of shapes for rapid recognition in real time.

3) Because opportunity (2) is a pattern-recognition problem that potentially involves a very large amount of data, there is a strong likelihood that machine learning techniques would be useful.

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

Research on campus will continue with colleagues in the mathematics department. We are planning, following more experimentation, to submit a grant to the NSF Archaeometry program this fall. This award will be used to support development of a machine learning initiative aimed at rapidly identifying acoustic responses in SONAR data, simultaneously expediting field data review and removing operator error in the detection of resonance.

This semester, I will organize efforts to collect acoustic signatures from different materials to begin building a database of acoustic signatures from materials aside from lithics. This research will be the foundation of an entirely separate publication on the resonant signatures of anthropogenic materials.

Finally, I will use the SONAR equipment purchased through this award to begin survey in the Tennessee River near Chattanooga. It is my hope that this work, supported by local agencies such as the Tennessee Valley Authority and Eastern Band of the Cherokee Indian Tribal Historic Preservation Office, will highlight and preserve cultural heritage currently obscured beneath the murky water of the Tennessee River. This research could spawn external funding and scholarly articles on the preservation of archaeological sites following deliberate site inundation, expand our understanding of the use of the Tennessee River over 16,000 years, and new methods for next-generation cultural resource management of interest to the US Army Corp of Engineers, Bureau of Reclamation, and Tennessee Valley Authority.

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

This research has attracted substantial attention from industry and government practitioners, who are closely following the development of this technology. Similarly, pre-eminent scholars in the field of submerged landscape studies are likewise closely monitoring its development and have taken note of the role UTC is now playing in cutting-edge research. As we continue this work, we will continue to raise our institutional profile, which will pay future dividends in scholarly activity, external funding, and student placement/employment after graduation.

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

As with any long-term research initiative, funding will always be a primary problem. As this research requires water-based logistics, the acquisition of a research vessel fit for this kind of work, as well as a continuing budget to offset maintenance and fuel costs of tow-vehicles and research vessels, would be the single most effective way of ensuring long-term success.

In Anthropology, I also face the reality that I am a single person and can only dedicate so much time to this work while balancing other duties at work and home. Thus, this program has inspired me to consider the pursuit of a graduate program in Anthropology at UTC, which I have begun forming a working group to explore. This kind of research is well suited for graduate studies, and I hope to move such a program to fruition in the coming years.

FINANCIAL ACCOUNTING

According to the most recent budget developed with Anna Lane, I came in $1600.37 under budget.

The primary budget problem with this award was the loss of Abi Arabshahi at the start of the award, to whom nearly 1/3 of the original budget was allocated. To re-allocate these funds, I consulted with Drs. Tony Skjellum and Mina Sartipi to receive approval to add more travel expenses, doubling the number of field trials we were able to conduct, and to acquire next-generation SONAR instrumentation to enhance UTC’s research capacity in this area, outline above.

```
#Hermand_replicate
import fenics as fe
from dolfin import *
from dolfin_adjoint import *

#gets rid of critical error by identifying backend error (targets specific
output .png)CJA
import sys
import matplotlib
matplotlib.use('Agg')

import matplotlib.pyplot as plt
import numpy as np
import mshr
import time
import math
import os
import csv
from csv import writer
from csv import reader
from petsc4py import PETSc
start = time.time()
#define variables
fM = 4500 # Hz (IV.B.1 sim)
tol = 1E-14
rho_w = 1000
rho_s = 1900
rho_m = 1500
rho_sub = 2100
rho_c = 1500
rho_f = 2300 #kg/m^3
cp_f = 8433 #m/s
cs_f = 5843 #typo? should be m/s
nx = ny = 50

# Time variables
#changed T to be based on dt and Number of steps CJA
dt = 6.25*10**-8; t = 0; T = dt*50000 # s (IV.B.1 sim)

# checking if the directory png_op exists or not.
if not os.path.exists("flint_1_rhoDIR"):
    os.makedirs("flint_1_rhoDIR")

#defining ....
def wave_speed(x):
    cp = conditional(gt(x,0),1500,conditional(gt(x,-.1), 1650,
conditional(gt(x,-.3),1500, conditional(gt(x,-.35),1500, conditional(gt(x,-
.5),1650, 1950))))) # wavespeed in m/s (Table I)
    return cp
def sec_wave_speed(x):
    cs = conditional(gt(x,0),0,conditional(gt(x,-.1), 110,
conditional(gt(x,-.3),50, conditional(gt(x,-.35),50, conditional(gt(x,-
.5),110, 600)))))
    return cs
```

```
rho = Expression('x[1] > 0 ? rho_w : (x[1] > -.1 ? rho_s : (x[1] > -.35 ?
rho_m : (x[1] > -.5 ? rho_s : rho_sub)))',degree = 0, rho_w=rho_w,
rho_s=rho_s, rho_m=rho_m, rho_sub=rho_sub)

pml = Expression('exp(-.5*x[0])', degree = 2)
pmlr = Expression('exp(.5*x[0])', degree = 2)

def kappa(x, xmin, xmax, pml_width):
    kappa = 0
    a = xmin + pml_width
    b = xmax-pml_width
    kappa = conditional(lt(x,a), pml, conditional(gt(x,b),pmlr,1))
    return kappa

#https://fenicsproject.org/olddocs/dolfin/1.6.0/python/demo/documented/subdo
mains-poisson/python/documentation.html
# Create classes for defining parts of the boundaries and the interior of
the domain
class Left(SubDomain):
    def inside(self, x, on_boundary):
        return near(x[0], -5.0)

class Right(SubDomain):
    def inside(self, x, on_boundary):
        return near(x[0], 5.0)

class Bottom(SubDomain):
    def inside(self, x, on_boundary):
        return near(x[1], -3)

class Top(SubDomain):
    def inside(self, x, on_boundary):
        return near(x[1], 2.0)
############################
class Flint1(SubDomain):
    def inside(self, x, on_boundary):
        return (between(x[1], (-.31,-.305)) and between(x[0], (-3.5, -3.4)))
        ##flint at (-3.5,-.31) to (-3.4,-.305)

class Flint2(SubDomain):
    def inside(self, x, on_boundary):
        return (between(x[1], (-.31,-.305)) and between(x[0], (-3.26, -
3.14)))
        ##flint at (-3.26, -.31) to (-3.14, -.305)

class Flint3(SubDomain):
    def inside(self, x, on_boundary):
        return (between(x[1], (-.31, -.305)) and between(x[0], (-2.94, -
2.86)))
        ##flint at (-2.94, -.31) to (-2.86, -.305)

# Initialize sub-domain instances
left = Left()
top = Top()
right = Right()
bottom = Bottom()
flint1 = Flint1()
```

```
flint2 = Flint2()
flint3 = Flint3()

# Define mesh
mesh = RectangleMesh(Point(-5, -3), Point(5, 2), nx, ny)


# Initialize mesh function for interior domains
domains = MeshFunction('size_t', mesh, mesh.topology().dim(),0)
domains.set_all(0)
flint1.mark(domains, 1)
flint2.mark(domains, 1)
flint3.mark(domains, 1)

# Initialize mesh function for boundary domains
boundaries = MeshFunction('size_t', mesh, mesh.topology().dim()-1)
boundaries.set_all(0)
left.mark(boundaries, 1)
top.mark(boundaries, 2)
right.mark(boundaries, 3)
bottom.mark(boundaries, 4)

q = Expression('exp(-.5)*sin(pi/2*x[1])', degree = 2)
p = dt  # arbitrary function can go here
f = Constant(0) #kg/(m*sec^2)
g = Constant(0)

# Define function space and basis functions
V=FunctionSpace(mesh, "Lagrange", 1)
u = TrialFunction(V)
v = TestFunction(V)

# Extracting spatial coordinates associated with the mesh
x, y = SpatialCoordinate(mesh)

# Previous and current solution
u1= interpolate(Constant(0.0), V)
u0= interpolate(Constant(0.0), V)

# Define Dirichlet boundary conditions at top and bottom boundaries
bcs = [DirichletBC(V, 0.0, boundaries, 4), DirichletBC(V, 0.0, boundaries,
1), DirichletBC(V, 0.0, boundaries, 2)]

# Define new measures associated with the interior domains and
# exterior boundaries
dx = Measure('dx', domain=mesh, subdomain_data=domains)
ds = Measure('ds', domain=mesh, subdomain_data=boundaries)

a = rho*u*v*dx(0) + rho*dt**2*((wave_speed(y))**2-
2*(sec_wave_speed(y))**2)*inner(kappa(x, -5, 5, .5)*grad(u), grad(v))*dx(0)
+ rho_f*u*v*dx(1) + rho_f*dt**2*(cp_f**2-2*cs_f**2)*inner(kappa(x, -5, 5,
.5)*grad(u), grad(v))*dx(1)
L = rho*2*u1*v*dx(0)-rho*u0*v*dx(0) + rho*f*v*dx(0)+rho_f*2*u1*v*dx(1)-
rho_f*u0*v*dx(1) + rho_f*f*v*dx(1)

A, b = assemble_system(a, L,bcs)
```

```
j = 0
u=Function(V)
dispf_vals = []
disp_vals = []
time_vals = []
while t <= T:
    A, b = assemble_system(a, L,bcs)

    ricker = (1 - 2*pi**2*fM**2*t**2)*math.exp(-pi**2*fM**2*t**2)
    delta = PointSource(V, Point(-3.5, .5), ricker)
    delta.apply(b)
    solve(A, u.vector(), b)
    coord = V.tabulate_dof_coordinates()
    u0.assign(u1)
    u1.assign(u)

    disp = u(Point(-2.9,.5))
    dispf = u(Point(-3.2, -.3075))
    t += dt
    j = j + 1
    if ( j % 100 == 0):
      label = 'Time = %g' % (t)
      plot ( u, title = label )

      plt.plot(-3.4,.5, 'r+', markersize = 2)
      plt.text(-3.5,.6,'H1')

      plt.plot(-2.9,.5, 'r+', markersize = 2)
      plt.text(-3.0,.6,'H5')

      plt.plot(-2.3,.5, 'r+', markersize = 2)
      plt.text(-2.5,.6,'H10')
#marking flints on graph even though they aren't there for no flint
      plt.plot(-3.5,-.31, 'ks',markersize = 3)
      plt.plot(-3.26, -.31,'ks',markersize = 3)
      plt.plot(-2.94, -.31,'ks',markersize = 3)


      plt.text(-3,-1,'Flints')
      plt.arrow(-3,-1,-.26,.7)
      plt.arrow(-3,-1,-.5,.7)
      plt.arrow(-3,-1,.06,.7)

#subdomain water/sand
      point1 = [-5, 0]
      point2 = [5, 0]
      x_values = [point1[0], point2[0]]
      y_values = [point1[1], point2[1]]
      plt.plot(x_values, y_values, 'k', linestyle="--")
```

```
#subdomain sand/mud
      point1 = [-5, -.1]
      point2 = [5, -.1]
      x_values = [point1[0], point2[0]]
      y_values = [point1[1], point2[1]]
      plt.plot(x_values, y_values, 'b', linestyle="--")

#subdomain mud/cultural
      point1 = [-5, -.3]
      point2 = [5, -.3]
      x_values = [point1[0], point2[0]]
      y_values = [point1[1], point2[1]]
      plt.plot(x_values, y_values, 'o', linestyle="--")

#subdomain cultural/sand
      point1 = [-5, -.35]
      point2 = [5, -.35]
      x_values = [point1[0], point2[0]]
      y_values = [point1[1], point2[1]]
      plt.plot(x_values, y_values, 'r', linestyle="--")

#subdomain sand/substrate
      point1 = [-5, -.5]
      point2 = [5, -.5]
      x_values = [point1[0], point2[0]]
      y_values = [point1[1], point2[1]]
      plt.plot(x_values, y_values, 'y', linestyle="--")

      filename = 'flint_1_rhoDIR/simple_wave_solution_%d.png' % ( j )
      plt.savefig ( filename )
      print ( '  Graphics saved as "%s"' % ( filename ) )
      plt.close ( )
    time_vals.append(t)
    disp_vals.append(disp)
    dispf_vals.append(dispf)
plt.xlim(0, .000125)
plt.ylim(-1200,200)
font = {'family': 'serif',
        'color':  'darkred',
        'weight': 'normal',
        'size': 16,
        }

headerList = ['time','pressure','flint']
with open('disp_flint_1_rhoDIR.csv', 'w') as outfile:
    dw = csv.DictWriter(outfile, delimiter = ',', fieldnames = headerList)
    dw.writeheader()
    for time_vals, disp_vals, dispf_vals in zip(time_vals, disp_vals,
dispf_vals):
        print(time_vals,",",disp_vals,",",dispf_vals, file=outfile)
outfile.close()

plt.xlabel('Time', fontdict = font)
plt.ylabel('Pressure', fontdict = font)
plt.title('Pressure at H5 over time flint', fontdict=font)
plt.subplots_adjust(left=0.2)
plt.scatter(time_vals,disp_vals, s=1)
```

```
filename = 'DisplacementH5 flintDIR'
plt.savefig ( filename )
plt.close  (  ) end = time.time()
time_diff = (end-start)/60
print(time_diff,'min')
```

Fiscal Year 2023 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Applied Computational Science and Engineering Grant Competition

Dr. Lani Gao, Lead PI

Co-PI(s): Dr. Negwan Zahry (Communication), Dr. Ziwei Ma (Mathematics)

Other Personnel: Gertrude Osei (graduate student worker), James Pritchard (undergraduate student worker)

Project Title: "Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy"

Date Submitted: 8/20/2023

Award Start – End Date: July 1, 2022 – June 30, 2023

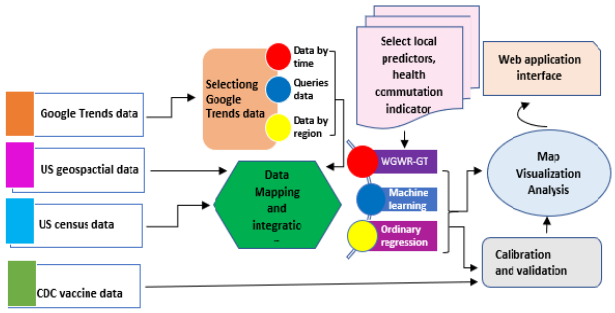
Non-Technical Summary:

We proposed a multiscale geographical weighted regression model integrated with Google Trends data analysis (MGWR-GT) to study CVH. MGWR-GT model accounts for common factors association with COVID vaccine hesitancy (CVH), as well as geographical and regional specifics of human behavior toward pandemic. The performance of MGWR-GT with be compared with machine learning methods including neural network, random forest, decision tree and traditional regression methods. Our preliminary study shows that the proposed model achieved more accurate estimation but with less bias subject responses. The predicted CVH rate can guide COVID vaccine administration and distribution efforts at the state and local levels with consideration of disparities such as race, ethnicity, gender, sexuality, socioeconomic status, age, geographic location, education level, disability status, immigrant status, health commutation and local policy and vulnerable populations. Moreover, reliable results given by the model would help public health decision makers respond to the public health crises more quickly, more efficiently, and more effectively. Furthermore, the proposed method can serve as a framework to predict human behavior toward public health crises by integrating traditional data and next-generation dynamic web search data. Finally, this research work will strengthen the real-time data analytics on health-related web queries in this big data era. Our project aims to achieve the following research goals:

- To examine and analyze the factors that influence vaccine hesitancy locally and globally.
- To assess the rate of COVID-19 vaccine acceptance, intention, and hesitancy locally and globally.
- To develop a conceptual framework of integrating seasonality of next-generation real-time dynamic data with traditional data analysis
- To explore the vital role of health communication in handling public health crises

PROJECT TITLE: “Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy”
Technology Area of Interest: Health & Biological Systems

TECHNICAL APPROACH	OUTCOMES
• multiscale geographical weighted regression model integrated with Google Trends data analysis (MGWR-GT) • Integrate multi data sources locally and globally. • Develop and employ Long Term Short Memory (LTSM) model. • developed workflow in R code.	• One conference paper was accepted and presented at Society of Risk Analysis conference (SRA) in Dec 2022. • One manuscript is submitted in June 2023 to the international Journal of Strategic Communication • A graduate thesis (Ms. Gertrude Osei) based on the project was successfully presented and accepted by graduate school of UTC in May 2023 • 2nd manuscript is ready to be submitted.

RESULTS	OTHER INFO
	**Budget and Schedule** • Total Budget: $95,577.00 • Actual Used: $87,119.66 • Balance: $8457.34 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** • One conference paper was accepted and presented at Society of Risk Analysis conference (SRA) in Dec 2022. • One manuscript is submitted in June 2023 to the international Journal of Strategic Communication. • A graduate thesis (Ms. Gertrude Osei) based on the project was successfully presented and accepted by graduate school of UTC in May 2023 • 2nd manuscript is ready to be submitted. • A poster presented at UTC Research and Art conference in April 2023 hosted by UTC graduate school. **Organization Information** UTC graduate school Phone: 423-425-4478

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
• Integrate Google Trend data. • Use classical statistics method VAR and Deep Learning method. • Build predictive models using proposed method (VAR)	The talk "*Predicting COVID-19 Vaccine Hesitancy through Analysis of Google Trends Data: Statistical Deep Learning Pilot Study"* was presented by PI Dr. Lani Gao at Southern Chapter Mathematics *Southeastern AMS Sectional Meeting at University of Tennessee at Chattanooga, Oct. 15-16, 2022.*
• Integrate communication Survey data from social media and employ Fear of Missing Out (FOMA) concept	Manuscript was accepted by Society of Risk Analysis (SRA) and it was presented by CO-PI Dr. Nagwan in Tampa FL in Dec 9 2021
• Neural network method was employed to the predictive model of COVID outcomes	"Predictive modeling of COVID outcomes Integrating google trend data" was presented at MATH Colloquium on Nov. 4th 2021
• Developed and validated proposed statistical VAR model	Dr. Gao's graduate student Ms. Gertrude Osei presented her master thesis successfully at UTC and thesis committed and graduate school approved afterwards in March 2023
• FOMO model with communication data via social media was employed in the predictive model	Manuscript "Optimizing Injunctive Norms to increase COVID-19 Vaccination Intention" was submitted to international Journal of Strategic Communication.

Challenges & Strategies Used to Address / Overcome:

The project faced hurdles stemming from the dynamic nature of online search behavior, data quality issues, and the representativeness of the Google Trends data. These challenges, while impeding the seamless achievement of proposed objectives and milestones, highlighted the importance of meticulous data preprocessing and the cautious interpretation of results in projects that rely on online search analytics for social phenomena analysis.

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

The project's initial expectation of a direct correlation between Google Trends data and vaccine hesitancy rates didn't hold true. The discrepancies highlighted the need for a more comprehensive and contextually informed approach, leading to a refinement of the project's

methodology and a valuable lesson in the importance of challenging assumptions, being open to unexpected outcomes, and adapting research strategies based on empirical evidence.

IMPACT & OUTCOMES

Impact on the Career(s) of the PI, the Co-PI(s), and Key Collaborators

The PI worked in a world leading childhood cancers research hospital environment before taking faculty position at UTC, which helped her gained valuable research experience in developing statistical methods, genetic and genome modeling and simulation in cancer research modeling and simulation of tumor growth. After joining UTC, the PI has been working closely with local hospitals and colleges of medicine on clinical trials, infectious disease, and cancer research. One Co-PI expertise in skewed sampling distribution, statistical modeling, and simulation. The third Co-PI is an expert in health communication, she has co-authored with PI on multiple papers and grant proposals. This pilot project will build an exciting collaboration between the PI and Co-PIs specialized in data analytics computing and modeling, and health communication and strategic communication via social media, and media with special focus on diversity issues. Led by this interdisciplinary team, the project aims to make transformative progress in the modeling and quantitative study of integration next-generation web-search data and traditional data.

Students Impacted

Two students were enlisted to actively contribute to the progress of this project. Ms. Gertrude Osei, a graduate student, received valuable support through the CVEACSE grant, where she served as a Research Assistant. Her master's thesis was intricately intertwined with the scope of this research initiative, forming a pivotal component of its execution. Upon the completion of her master's degree, her involvement in this research played a significant role in her successful acceptance into the PhD program in Biostatistics at Indiana University Purdue University Indianapolis in July 2023, underscoring the positive impact of this research experience on her academic journey. The second student, Mr. James Pritchard, an undergraduate, also found great value in this research endeavor. His participation contributed to his successful admission to the master's program at the University of Michigan, signifying the project's role in shaping and bolstering students' academic trajectories.

Community and Broader Impacts

The analysis of online search queries has been of notable popularity in the field of big data analytics in academic research (Preis 2012, 2013, Burnap 2015, Murray 2016). Web-based behavior is monitored and analyzed in order to examine actual human behaviors for accuracy prediction, better assessment, and possibly early prevention of public health related issues. Employing Google Trends data to analyze human behavior is a relatively novel practice. Google Trends has been proven valuable in examining seasonal trends in various diseases (Brigo 2015, Scheres 2016, Bragazzi 2016) and health issues such as the currently still spreading COVID-19, and cancer diseases (Rosenkrantz 2016). With integration of real-time social medial data online, the framework to be created in this research will have a broad applications of monitoring human behavior related to the public health.

Scholarly Products

Publications:

- *"*Optimizing Injunctive Norms to increase COVID-19 Vaccination Intention" was submitted to International Journal of Strategic Communication in June 2023.

- "Effective COVID-19 Outcome Modeling Using Google Trends Data: A Vector Auto Regression Approach" to be submitted.

External Conferences:

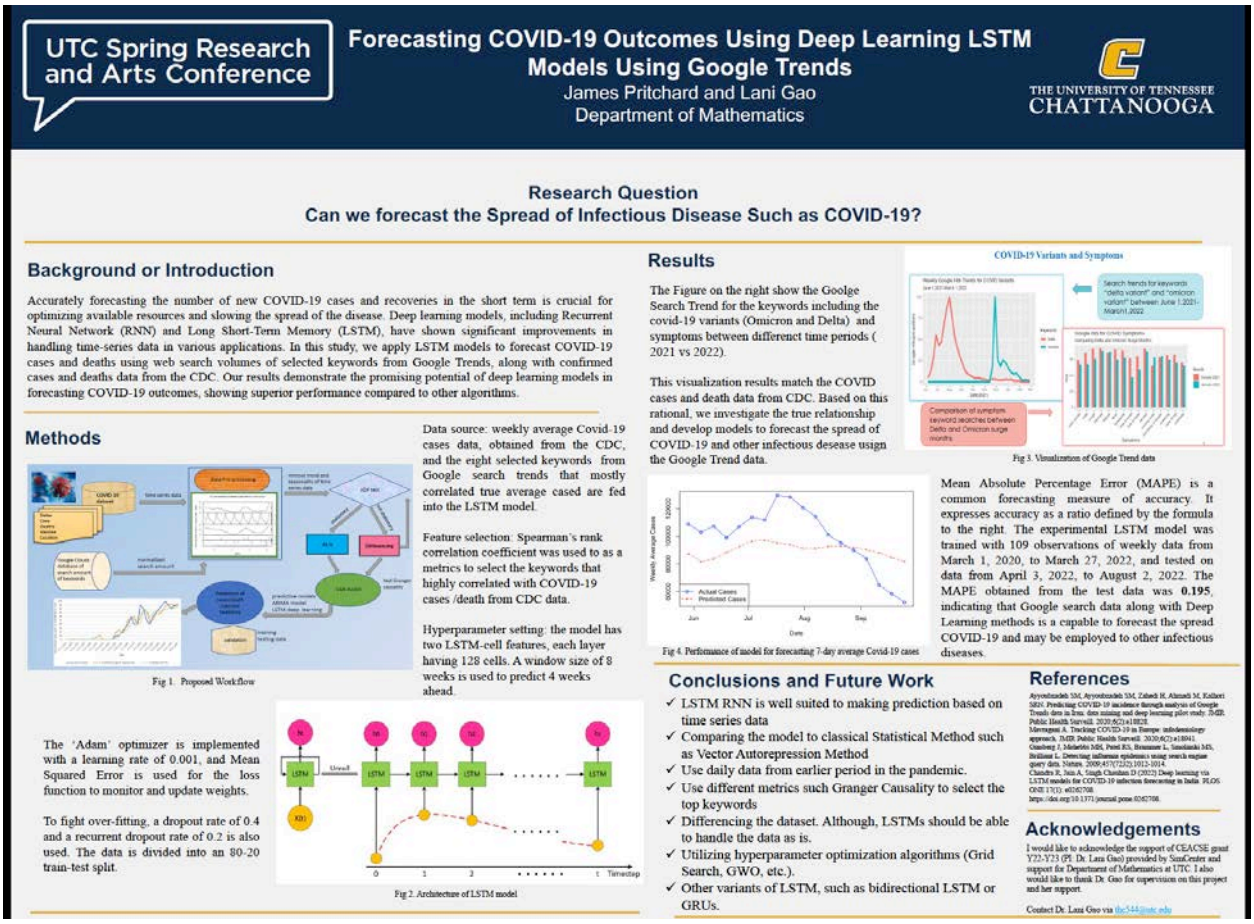
- The talk "Predicting COVID-19 Vaccine Hesitancy through Analysis of Google Trends Data: Statistical Deep Learning Pilot Study" was presented by PI Dr. Lani Gao at Southern Chapter Mathematics Southeastern AMS Sectional Meeting Oct. 15-16, 2022.

- "Forecasting COVID-19 Outcomes Using Deep Learning LSTM Models with Google Trends" was presented at conference Symposium on Data Science and Statistics in May 2023.

Presentations at UTC:

- "Predictive modeling of COVID outcomes Integrating google trend data" was presented by Dr. Lan Gao at MATH Colloquium on Nov. 4th, 2022.

- Poster "Forecasting COVID-19 Outcomes Using Deep Learning LSTM Models Using Google Trends" was presented by James Pritchard and Dr. Lan Gao in April 2023.



Inventions or Other Intellectual Property

An open-source R package for the proposed workflow in under preparation.

Research Outreach & Collaboration

We will collaborate with some researchers in computer science to seek external funding in the future.

EXTERNAL FUNDING

Proposal Submissions

- We planned to submit a proposal to NSF in Nov. 2023

Contracts/Awards Received

- None.

Sponsored Program Capacity Building Activities

The PI Dr. Lan Gao had applied for the NSF program solicitation Internet Measurement Research (IMR): Methodologies, Tools, and Infrastructure (IMR) webinar in Dec 2022.

WHAT'S NEXT FOR THIS RESEARCH?

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

Following the completion of the CEACSE grant-funded project "Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy," the research will enter an exciting phase of expansion, refinement, and application over the next 1 to 5 years. In the immediate year ahead, the research team will focus on publishing the project's findings in reputable academic journals and presenting them at relevant conferences. This dissemination will help establish the project's contributions to the field, sharing insights gained from the hybrid model and its implications for understanding vaccine hesitancy dynamics more accurately.

Over the subsequent 2 to 3 years, the research will involve collaborations with public health agencies, policymakers, and healthcare practitioners. The refined hybrid model, which incorporates Google Trends data, demographic factors, and community insights, will be utilized to inform targeted interventions and communication strategies aimed at addressing vaccine hesitancy at local levels. This applied phase of the research will involve close engagement with communities, utilizing the insights gained to tailor education campaigns and outreach efforts that resonate with specific populations.

In the longer term, spanning the next 4 to 5 years, the research will contribute to the establishment of a comprehensive framework for understanding and combating vaccine hesitancy. This framework will integrate diverse data sources, account for varying sociocultural contexts, and provide actionable insights to guide vaccination programs globally. Additionally, the project's success may inspire similar interdisciplinary endeavors in addressing other complex societal challenges, fostering ongoing collaborations between data scientists, social scientists, healthcare professionals, and policymakers. Overall, the research's journey will evolve from data analysis and model development to meaningful impact on public health practices and societal well-being.

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

I would also like to pursue the NSF grant "Smart Health and Biomedical Research in the Era of Artificial Intelligence and Advanced Data Science (SCH) program".

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?

One barrier is to find the appropriate collaborator in computer science who will help build the flow work of the integrated model as well as understand the statistical learning algorithm.

FINANCIAL ACCOUNTING

I had to cancel a registered conference at St Louis between May 23-26 due to my father's pass away on May 20 member's death and I had to fly back to China, which cause some travel money budgeted left. In addition, one student worker had to leave the project as he found a job at NASA, which caused a few hundred left for payment for students.