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 2022

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Submitted by
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THE UNIVERSITY OF TENNESSEE CHATTANOOGA

SIMCENTER

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

MISSION STATEMENT

To establish, expand, and sustain a cohesive multidisciplinary effort in applied computational sciences 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 2022 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 21st year in Fall 2022.

With our previous report for FY2021, CEACSE marked its 19th 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 FY2022 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 FY2022 include these highlights:

- SimCenter is a partner, together with the University of Alabama, on the DOE/NNSA Center led by the University of New Mexico – Center for Understandable, Performant Exascale Communication Systems, which provides national center recognition and funding to our efforts in high performance computing. Dr. Skjellum is a co-PI of this effort, which extends through the end of FY2025, with potential for renewal.
- PI Azad Hossain's project led to one externally funded project following on to this work.
- PI Loren Hayes was promoted to full professor.
- PI Hossain was promoted to Associate Professor and received tenure.
- PI Sungwoo Yang received $100,000 of follow-on funding from the State of California to work on insulating materials to improve energy efficiency.

- PI Eleni Panagiotou and co-PI Jin Wang submitted and were awarded an NSF grant to work on follow-ons to their CEACSE-funded project. They also established a new collaboration with ORNL in the framework of this grant.
- PI Hamdy Ibrahim was first-place winner in UTC's Inaugural "Fly for Researchers" competition, providing him with $20,000 of support to commercialize research related to his CEACSE award.
- SimCenter placed two undergraduate students at DOE Laboratories – Pacific Northwest National Laboratory (PNNL) and Lawrence Livermore National Laboratory (LLNL). Two students, including one of these interns, received job offers from LLNL.
- Former PI Hong Qin received recognition from the National Academic of Medicine for work on an earlier CEACSE award; this work also leveraged SimCenter computational facilities. Dr. Qin was awarded $50,000 in this round of recognition for his submission entitled "Uncovering molecular mechanisms of aging clocks with interpretable deep learning."
- In collaboration with Tennessee Tech, SimCenter hosted the second of two workshops on Digital Twin engineering curriculum, funded by the National Science Foundation. The first workshop was held virtually in FY2021 at UTC during the COVID-19 pandemic.

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 2022 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 FY2022 budget and expenditures for FY2022, as well as outyear requests.

In Memoriam

We are sorry to report that our colleague, Dr. Mark Schorr, a co-PI on one of the CEACSE efforts, passed away during FY2022. He is sorely missed by his colleagues in the College of Arts and Sciences and others who knew him.

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FACULTY & STAFF

The Center of Excellence in Applied Computational Science and Engineering benefits from institutional leaders who are deeply committed to enriching and expanding computational science as a research area and as an enabler of innovative research across academic departments. The THEC Chair of Excellence is Dr. Tony Skjellum. 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 FY2022 Awardees

The following faculty and staff were integral to the strategic direction of CEACSE during the 2021–2022 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. Yunye Shi

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

Lead PI: "Predicting Biomass Gasification Output – A Machine Learning Approach"

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.

Lead PI: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"

Dr. Jejal Bathi

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

Co-Investigator: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"

Dr. Mark Schorr

Mark Schorr received his BS in Zoology from Southeastern Louisiana University, his MS in Zoology from Mississippi State University, and his PhD in Forest Resources (Fisheries Management) from Mississippi State University. His primary research interest is stream fish ecology, with an emphasis on water pollution issues and population/community ecology. Graduate and undergraduate students working in his laboratory have conducted research to address the following problems: (1) influence of coal mine drainage on stream water chemistry, habitat, and aquatic macrofauna (macroinvertebrates, fishes, salamanders) in the Cumberland Plateau; (2) landscape-stream relationships that involve watershed land use, riparian buffers, limnological parameters, and macrofaunal assemblages in Ridge and Valley catchments; (3) localized effects of road culverts on instream habitat and fish assemblages in Blue Ridge catchments; (4) lotic macrofaunal responses to stream restoration projects (artificial pools/riffles, constructed channels); and (5) historical and contemporary patterns in the distribution and abundance of the introduced redbreast sunfish (Lepomis auritus) and native congeneric sunfishes (Lepomis spp.; Centrarchidae) in reservoirs in the Tennessee River drainage.

Co-Investigator: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"

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: "Corrosion Modeling of Magnesium-based Fixation Hardware for Mandibular Reconstruction Surgeries"

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.

Co-Investigator: "Corrosion Modeling of Magnesium-based Fixation Hardware for Mandibular Reconstruction Surgeries"

Dr. Loren Hayes

Dr. Loren Hayes is an Associate Professor in Biology, Geology and Environmental Science. He received his BS in Biology from Bates College, MS in Zoology from Michigan State University, and PhD from Miami University. His research interests include the fitness consequences of communal living and the drivers of social evolution in mammals. He has 50 publications in a range of internationally reputable journals, including Animal Behavior, Behavioral Ecology, Biology Letters, Ethology, Journal of Mammalogy, Trends in Ecology and Evolution, and Proceedings of the Royal Society B. He has published numerous book chapters and co-edited a book on the sociality of caviomorph rodents. He regularly presents his research at

international conferences and is co-host of a remote, international seminar series on social evolution. He has generated nearly $1 million in research funding, mostly from NSF.

Lead PI: “Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models”

Dr. Jin Wang

Dr. Jin Wang is Professor and UNUM Chair of Excellence in Applied Mathematics at UTC. He obtained his PhD in Computational and Applied Mathematics from The Ohio State University in 2004. Before joining UTC, he worked at Duke University and Old Dominion University. His research interests include mathematical modeling, numerical analysis, scientific computing, mathematical biology, and fluid dynamics.

Co-Investigator: “Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models”

Dr. Mina Sartipi

Mina Sartipi is the Founding Director of the Center for Urban Informatics and Progress (CUIP) and is also a Guerry Professor in the Computer Science and Engineering Department, where she leads the Smart Communications and Analysis Lab (SCAL). She received her BS in Electrical Engineering from Sharif University of Technology, Tehran, Iran, in 2001 and her MS and PhD degrees in Electrical and Computer Engineering from Georgia Tech in 2003 and 2006, respectively. She is a member of technical program committee for several workshops and conferences on topics related to AI and smart city operations. She was named 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 is recipient of several awards including 2016 UT-Chattanooga Outstanding Faculty Research and Creative Achievement award, UC Foundation Professorship, and 2020 Smart 50 awards in Digital Transformation at the Smart Cities Connect (in collaboration with CHA and EPB). She has published over 50 papers related to data science, wireless communications, connected vehicles, and data integration. She has delivered several keynotes and presentations including US Congressional Caucus on Smart Cities, live demo of connected vehicle project at the Smart City Connect, and National Transportation Training Directors. Dr. Sartipi has been an IEEE senior member since 2016. She is a member of the Board of Directors for the Enterprise Center, Chattanooga, TN, Variable, Inc., Thrive Regional Partnership, and Mohuman. Dr. Sartipi’s research interests are in the area of wireless communications and data analysis for smart city applications including mobility, health, and energy. Her research is supported by NIH, NSF, DOE, State of TN, foundations, and industry.

Lead PI: “Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications”

Dr. Farah Kandah

Dr. Farah Kandah is an IEEE Senior Member and a UC Foundation Associate Professor in the Computer Science and Engineering (CSE) department at the University of Tennessee at Chattanooga (UTC). He is leading the Cybersecurity and Cyber-Physical Systems thrust at the SimCenter, leading the Network Communication Laboratory (NCL) at UTC, and co-leading the IoT laboratory at the SimCenter. His research focuses on smart communications to support real-time interactions in wired and wireless networks, threat hunting, Blockchain, and trust management in areas of Internet of Things, Smart networking design, Smart Connected Vehicles, Cybersecurity, Cyber-physical systems, and Software-Defined Networks. He has served as a technical committee member, a Co-Chair, and a Session Chair for conferences in the field of wireless communications and networking such as CHINACOM, IEEE ICNC, and IEEE CCNC. He has also served as a reviewer for international journals including the Security and Communication Networks, IEEE Sensor Networks, and the International Journal of Information Processing and Management (IJIPM).

Co-Investigator: "Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications"

Dr. Osama Osman

Dr. Osman is formerly the Assistant Professor of Intelligent Transportation Systems and Data Analytics in the Department of Civil and Chemical Engineering (CCE) at the University of Tennessee at Chattanooga (UTC). Prior to joining UTC, he was a research faculty at the Center for Sustainable Mobility at Virginia Tech Transportation Institute (VTTI).

His research interests span intelligent transportation systems, traffic operation and control, connected vehicle (CV) and connected autonomous vehicle (CAV) technologies, computer and human-in-the-loop simulation, traffic safety and human factors, and application of artificial intelligence, machine learning, and deep learning in transportation. Particularly, his research focuses on mathematical and simulation modeling and analysis of CV and CAV environments, application of advanced modeling and data analytics techniques for traffic control and congestion management, developing machine learning and deep learning algorithms for detection and prediction of risky driving behavior, and investigation of impact of emerging vehicular technologies and smart mobility on mobility, energy, and behavioral safety. He authored or co-authored over 60 publications in peer-reviewed journals, national and international conference proceedings, technical reports, and a book chapter. He is also the recipient of the 2020 best paper award on User Information Systems from the Transportation Research Board of the National Academies of Sciences.

Co-Investigator: "Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications"

Dr. Stephanie DeVries

Dr. Stephanie DeVries is an assistant professor in the department of Biology, Geology and Environmental Science. She received her PhD from City College of New York Graduate Center in Earth/Environmental Science in 2017. Her research interests fall into three broad categories: occurrence and impacts of emerging contaminants on terrestrial and aquatic ecosystems; agricultural management systems and water quality and policy; and land-atmosphere exchange of nitrogen under changing climate conditions.

Lead PI: "A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers"

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.

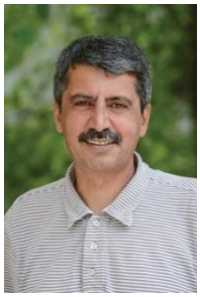
Lead PI: "A study on the local and global effects of polymer entanglement in material properties and biological functions"

Dr. Wang-Yong Yang

Dr. Wang-Yong Yang is an Assistant Professor of Chemistry at the University of Tennessee, Chattanooga. He earned his Bachelor/Master of Science in Chemistry at Pusan National University, Korea, in 1996/1998 and joined Dong-Wha Pharmaceutical Ind. Co., Korea as a researcher. For 6 years in the company, he focused on two projects: 1. Development of Non-nucleoside HBV & HCV Inhibitor, 2. Development of Potent Quinolone Class Antibiotics. He moved to USA and received his PhD in Organic Chemistry from Florida State University, Tallahassee in 2011, working with Prof. Igor Alabugin. His thesis work was Design of pH-Controlled Light-Activated Reagents for Efficient Cleavage of Double-Stranded DNA and Cancer Phototherapy. After completing his PhD, Yang started his postdoctral fellowship in the Scripps Research Institute in Jupiter, FL, under supervision of Dr. Matthew Disney. During that time, he developed Small Molecules Targeting Toxic RNAs related to Human Neurodegenerative Diseases such as Fragile X-associated tremor/ataxia syndrome (FAXTAS) and spinocerebellar ataxia-10 (SCA10). In 2018, Yang accepted an Assistant Professor position at University of Tennessee, Chattanooga.

Co-Investigator: "A study on the local and global effects of polymer entanglement in material properties and biological functions"

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: “A study on the local and global effects of polymer entanglement in material properties and biological functions”

FY2022 STUDENTS

Project Title: Predicting Biomass Gasification Output – A Machine Learning Approach

Lead PI: Dr. Yunye Shi

Students Impacted:

Brenan Ward: The student worked on the project for over 3 months and developed a basic understanding of machine learning. Brennan is seeking further opportunities to stay in the team for graduate study.

Hannah Morgan: The student was introduced to the project during her junior year and did data analysis for the project.

Greg Johnson: The student worked on the project during his senior year (Fall 2021—Spring 2022). He has converted the code developed in R into Python. During the process, the student successfully used the coding skills he learned from class into a new topic. He presented the work at both UTC Tech Symposium and NCUR.

Project Title: Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies

Lead PI: Dr. Azad Hossain

Students Impacted:

Richard Blanton: Mr. Blanton is a graduate (MS) student in the Environmental Science program. He graduated in December 2019. He is currently working as a term research assistant for this project. He has been involved in water quality remote sensing research in the Geological and Environmental Remote Sensing (GERS) Laboratory at UTC for more than a year. This project provides him with the opportunity to continue participating in this research and experience how it can be integrated with numerical hydrodynamic and watershed models. This unique research experience helps him to become ready for pursuing further higher education and/or starting professional or research careers in this area. Recently Mr. Blanton has assumed a GIS Analyst position at the Tennessee Valley Authority (TVA). Before joining the TVA, he worked at the GIS Department of Hamilton County, TN.

Caleb Mathias: Mr. Mathias is a recently graduated undergraduate student in Geology. He joined GERS Laboratory at UTC at the beginning of fall 2019 as a term research assistant for this project. This project provides him with the opportunity to conduct water quality remote sensing research and how it can be integrated with numerical hydrodynamic and watershed models. He is gaining valuable post baccalaureate research experience through this project. This unique research experience helps him prepare for pursuing higher education and/or starting professional or research careers in this area. Mr. Mathias has been admitted in the graduate program at the University of British Columbia (UBC) in Canada with full research assistantship. He will join UBC in fall 2021.

Connor Firat: Mr. Connor Firat is a graduate (MS) student in the Environmental Science program. He is currently working on his thesis research that integrates remote sensing technology with hydrodynamic models to estimate water quality parameters in the Tennessee River and adjacent creeks. He has been involved in water quality remote sensing research in the Geological and Environmental Remote Sensing (GERS) Laboratory at UTC for more than a year.

Abbie Faxon: Ms. Abbie Faxon is a recently graduated undergraduate student in Geology. Abbie graduated in Spring 2022 with a major in Geology and minor in Geographic Information Systems (GIS). Abbie successfully defended her Departmental Honors Thesis on remote sensing of water quality. She used this project's resources to analyze water samples for estimating total suspended sediments (TSS). Abbie recently accepted a position in the remote sensing division of the Oak Ridge National Laboratory (ORNL).

Shuvashish Roy: Mr. Roy joined this project as a graduate (MS) student in Civil Engineering. He graduated in May 2020 and recently joined the industry as an engineer. He was instrumental for the development of the EFDC 3D hydrodynamic model for part of the Tennessee River.

Syed Tareq: Mr. Tareq joined this project as a graduate (MS) student in Civil Engineering. He also graduated in May 2020 and started pursuing a PhD in Computational Engineering at UTC. He was also involved in the development of the EFDC 3D hydrodynamic model for part of the Tennessee River.

Project Title: Corrosion Modeling of Magnesium-based Fixation Hardware for Mandibular Reconstruction Surgeries

Lead PI: Dr. Hamdy Ibrahim

Students Impacted:

Moataz Abdalla, graduate student: He was completely funded and led the students' effort in this project for one year. He is expected to graduate spring 2021.

Austin Sims, graduate student: He was partially funded in this project. He is expected to graduate fall 2020.

Alexander Joplin, undergraduate student: He was partially funded in this project during spring and summer 2020.

Clay Jones, undergraduate student: He was partially funded in this project during spring 2020

Project Title: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models

Lead PI: Dr. Loren Hayes

Students Impacted:

Elizabeth Pope: environmental science, M.S.: Pope analyzed life history data and contributed to a UTC Research Dialogues poster. She did an excellent job with the analysis and trained several other students. She left the M.S. program to pursue other goals.

Evan Suggs: computerscience, M.S.: Suggs worked on machine learning projects and is entering his second year of the M.S. program. He had a change in PI due to the departure of Tanis from UTC.

Braxton Azalone: geology, undergraduate: Azalone is working on a rainfall dataset in summer 2021. He plans to graduate in 2022.

Madison Roberts: biology, undergraduate: Roberts is working with Schradin on a related project and is supported by NSF IRES. She was not funded by CEACSE. She plans to continue her project into fall 2021, leading to an honors thesis.

Madeline Townsend: biology, undergraduate: Townsend worked on a related project (Cetacean social organization) but was not funded by CEACSE. She graduated from UTC inspring 2021.

Logan Platt: ESC, graduate student: Worked with a colleague in Colombia to prepare a large dataset for future collaboration (using R).

Project Title: Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications

Lead PI: Dr. Mina Sartipi

Students Impacted:

Jewel Rana Palit: supported by the grant as a MS student.

Jibril Babatunde: partially supported by the grant as a MS student.

Faiza Khan: partially supported by the grant as a MS student.

All students are supported by the grant at different stages. All students involved in this project gained experience in simulation technologies and VR development

Project Title: A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers

Lead PI: Dr. Stephanie DeVries

Students Impacted:

Gavin Hasty, Geology (’21): Developed skill using Rockworks to prepare borehole logs and develop a 3D geologic model. This software is widely used in geologic research and consulting and the student will benefit from this experience his professional future.

William (Garrett) Hooten, Computer Science (’22): Programmed a stand-alone program that calculates the concentration of a contaminant well water as a function of land use using input data from USDA CropScape and a 3D groundwater flow model. Student gained valuable experience programming a practical application and will be featured as 2nd author on a pending publication.

Matthew Mollica, Geology (’23): Created input data for simulations that tested the effect of different crop rotations on groundwater nitrate concentrations in a study well. Ran the model for each set of scenarios and created appropriate figures to communicate the results. The student will be featured as 3rd author on a pending publication.

Project Title: A study on the local and global effects of polymer entanglement in material properties and biological functions

Lead PI: Dr. Eleni Panagiotou

Students Impacted:

Evan Gildernew, participated in research and gave poster presentation, graduate student, MS Chemical Engineering.

Peter Zeglen, participated in research, graduated Bachelor in Mathematics.

Tanner Smith, initial training in research, PhD student in Mathematics (not funded by the grant due to insufficient interest and commitment).

Matthew Phanner, participating in research, Bachelor in Chemistry.

Justin Pease, participating in research, Bacelor in Chemistry.

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.

FY2022 has been another year of growth and enhancement for CEACSE. The leadership team comprises Drs. Joanne Romagni (Vice Chancellor for Research) and Tony Skjellum (SimCenter Director). Strong collaborative interactions with UTC faculty and administrators underpin this program.

Dr. Skjellum has led the CEACSE efforts for five years as of the date of this report, and he plans to continue to grow and support work consonant with the original proposal to THEC for CEACSE. Continued emphasis on modeling and simulation in CSE, HPC/HPT, and data science ground the strategy of advancing and diversifying the participation of UTC faculty and students in CEACSE projects in FY2023 and beyond.

The FY2022 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 FY2022 include these highlights:

- SimCenter is a partner, together with the University of Alabama, on the DOE/NNSA Center led by the University of New Mexico – Center for Understandable, Performant Exascale Communication Systems, which provides national center recognition and funding to our efforts in high performance computing. Dr. Skjellum is a co-PI of this effort, which extends through the end of FY2025, with potential for renewal.
- PI Azad Hossain's project led to one externally funded project following on to this work.
- PI Loren Hayes was promoted to full professor.
- PI Hossain was promoted to Associate Professor and received tenure.
- PI Sungwoo Yang received $100,000 of follow-on funding from the State of California to work on insulating materials to improve energy efficiency.
- PI Eleni Panagiotou and co-PI Jin Wang submitted and were awarded an NSF grant to work on follow-ons to their CEACSE-funded project. They also established a new collaboration with ORNL in the framework of this grant.
- PI Hamdy Ibrahim was first-place winner in UTC's Inaugural "Fly for Researchers" competition, providing him with $20,000 of support to commercialize research related to his CEACSE award.

- SimCenter placed two undergraduate students at DOE Laboratories – Pacific Northwest National Laboratory (PNNL) and Lawrence Livermore National Laboratory (LLNL). Two students, including one of these interns, received job offers from LLNL.
- Former PI Hong Qin received recognition from the National Academic of Medicine for work on an earlier CEACSE award; this work also leveraged SimCenter computational facilities. Dr. Qin was awarded $50,000 in this round of recognition for his submission entitled “Uncovering molecular mechanisms of aging clocks with interpretable deep learning.”
- In collaboration with Tennessee Tech, SimCenter hosted the second of two workshops on Digital Twin engineering curriculum, funded by the National Science Foundation. The first workshop was held virtually in FY2021 at UTC during the COVID-19 pandemic.

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 FY2022/FY2023 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 FY2022 Projects

For FY2022, 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 FY2022: 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: Predicting Biomass Gasification Output – A Machine Learning Approach
Lead PI: Yunye Shi
Co-PI(s): N/A
*** This project was extended from FY2020, and was closed in 2022.***

Summary: Biomass gasification has been regarded as a promising technology to utilize bioenergy sustainably. Accurately predicting the outcomes of this process is a crucial step to achieve efficient design and optimal operations. For this purpose, various kinetics an equilibrium models are developed. However, the assumptions made in these models significantly limit the practical usability and consistency. The proposed research evaluates the performance of syngas output prediction using classical machine learning methods and establishes a novel recurrent neural network (RNN) framework. The RNN model is composed of a set of subnetworks. The transient behavior of each key step output is a function of the input parameter of the fixed-bed gasifier. The model will be trained with a large data set and validated with experimental data and other models.

Core Competition

Project Title: Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies
Lead PI: Azad Hossain
Co-PI(s): Jejal Bathi, Mark Schorr
*** This project was extended from FY2020, and was closed in 2022.

Summary: Satellite observations have been used for water quality studies for many years, but they provide only surface observations and challenges related to cloud coverage and ground truthing, and variable spatial and temporal resolutions remain. Numerical models can provide hydrodynamically computed water quality data on the water surface as well as in the water column, but they have issues with initializations, boundary conditions, calibration, and validation. Although both methods have weaknesses, when used together, they can become a powerful tool to study surface water quality. The proof of concept of this capability was demonstrated in Enid Lake, MS, Lake Pontchartrain, LA, and the Mississippi River using CCHE2D Flow and Water

Quality models developed in the National Center for Computational Hydroscience and Engineering at the University of Mississippi. The proposed study aims to further explore this capability at the University of Tennessee at Chattanooga by using the EPA's Better Assessment Science Integrating Point and Non-point Sources (BASINS) model coupled with NASA's Earth observation satellite imagery and near-real-time field measurements to study the spatio-temporal variability of hydrodynamically computed surface water quality parameters in the watersheds of southeast Tennessee.

Project Title: Corrosion Modeling of Magnesium-based Fixation Hardware for Mandibular Reconstruction Surgeries
Lead PI: Hamdy Ibrahim
Co-PI(s): Mohammad Mahtabi
*** This project was extended from FY2020, and was closed in 2022.

Summary: The long-term objective of this research is to develop biodegradable (nonpermanent) magnesium-based bone implants with suitable mechanical, physical, and biological properties to address the drawbacks of the currently-in-use permanent bone implants. This funded project succeeded in developing a subroutine and a model to predict the corrosion rate of biodegradable magnesium-based alloys for their biomedical applications. This model was calibrated by conducting a series of tests in conditions simulating the body environment. The findings of this study increased the knowledge on the biomechanical performance of biodegradable magnesium-based materials. The project has also enhanced the infrastructure for research and education by increasing the level of current activity in the area of biomaterials. Four students (2 graduate and 2 undergraduate) were trained through this project in corrosion modeling, experimental corrosion testing, microstructural characterization, and mechanical testing. Several corrosion testing tools and devices were purchased from this project that will be available, for the first time, to faculty and students at the UTC to test the corrosion characteristics of metals and alloys.

Project Title: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models
Lead PI: Loren Hayes
Co-PI(s): Jin Wang
This project was postponed to FY2022, due to issues resulting from COVID-19.

Summary: A fundamental goal of biology is to understand the evolution of animal social systems. Comparative studies have failed to account for intraspecific variation in social organization (e.g., a species may live in groups or alone in different populations). Accounting for intraspecific variation in comparative studies is critical because the ability to change social organization may improve species resilience in the face of climate change. We aim to: (i) build a dataset on mammalian social organization that accounts for intraspecific variation and (ii) conduct a preliminary analysis to determine the impact of rainfall and temperature trends on artiodactyl social evolution. We focus on artiodactyls because the PI has completed manual data collection for this Order. We will conduct a semantic analysis of the literature, applying machine learning techniques to improve the consistency and speed of data collection (aim 1). We will use classical regression methods and machine learning–based predictive methods to test the hypothesis that variable rainfall and temperature are associated with variable social organization (aim 2). We will use the results of this study to strengthen a National Science Foundation proposal to conduct a comparative analysis of how climatic variation influences the evolution of mammalian (~5,500 species) social organization.

Project Title: Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications
Lead PI: Mina Sartipi
Co-PI(s): Farah Kandah, Osama Osman
This project was extended into FY2022, due to issues resulting from COVID-19.

Summary: The proposed research includes modeling, simulation, and computational performance analytics and optimization. The proposed research aims to enable application of Virtual Reality (VR) in a multi-player game setting for a wide spectrum of research applications at the University of Tennessee at Chattanooga. Specifically, an integrated multidisciplinary human-in-the-loop simulation platform will be developed to enable studying micro-level interactions between multiple heterogeneous road users in a VR multi-player setting. The research objectives are to: (a) develop an integrated simulator for heterogeneous road users that capitalizes on VR technology; (b) develop a behavioral data collection and visualization tool for the integrated simulator; and (c) demonstrate the capabilities of the integrated platform. The proposed integrated simulation platform will enable experimental research and training in highly controllable conditions. Additionally, the integrated platform will combine the advantages of various research methods: pedestrian-in-the-loop simulation for testing of pedestrian behavior in a wide range of applications, driver-in-the-loop simulation for experimental investigation of driver behavior in various scenarios, and data analytics and visualization techniques of behavioral data. The integrated platform will add a high degree of realism since assumptions and mathematical models of road user behaviors will not be the basis of simulation.

Project Title: A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers
Lead PI: Stephanie DeVries
Co-PI(s): N/A
*** This project was extended from FY2020, and was closed in 2022.

Summary: The original objective of this project was to evaluate a novel method for digitizing a homogeneous glacial aquifer for 3-dimensional groundwater flow modeling. The model is based on a statistical tool called Thiessen Polygons and can be produced quickly using data reported on well construction reports. More traditional methods of subsurface digitization include statistical models or development of a geologic framework model, which require significantly more expertise and time, which makes groundwater flow modeling cost-prohibitive for some applications. This project aimed to demonstrate that the Thiessen Polygon method yielded statistically comparable results when incorporated into a 3D groundwater flow model.

Project Title: A study on the local and global effects of polymer entanglement in material properties and biological functions

Lead PI: Eleni Panagiotou
Co-PI(s): Jin Wang, Wang-Yong Yang, Abi Arabshahi
*** This project was extended from FY2020, and was closed in 2022.

Summary: This proposed research is focused on making the connection between microscopic and macroscopic properties in polymers and biopolymers. First, we propose to use Molecular Dynamics (MD) simulations of coarse-grained models of linear polymer chains in a melt, for various molecular weights and examine how the entanglement affects the mechanical properties of the material. We will also examine the role of the fluid-structure interactions, and our results

will be compared to experimental data. Our results will show how local/global interactions affect material properties, a fundamental question in materials science and in the study of biological systems like the cytoskeleton. Second, we propose to use MD simulations of RNA, which include expanded r(AUUCU) repeats (responsible for spinocerebellar ataxia) to identify special characteristics of their 3D structure. We also study the dimeric compound 2AU-2 that is known to target the pathogenic RNA and model its binding by accounting for fluid-structure interactions. We use topology to study these and to suggest other molecules that would have the same effect. We check our results experimentally. Our results will show how geometry/ topology can be used to create site-specific molecules and could be applied to other extended repeats and lead to site-specific drug delivery methods.

FY2022 Budget

NEW CORE AWARDS FY2022				
Lead PI	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Fernado Alda	Identification and Prediction of Species Invasiveness Potential in the Gut Microbiome	Health and Biological Systems	$90,000	$32,850**
David Giles	From *in vitro* to *in silico*: Exploring the Therapeutic Potential of Antimicrobial Peptides on Exogenous Fatty Acid Modification of Bacterial Membranes	Health and Biological Systems	$99,926	$66,866**
Hamdy Ibrahim	Degradation Modeling of Coated Magnesium Towards Patient-Specific Biomedical Implants	Health and Biological Systems and Advanced Modeling and Simulation	$95,111	$14,924**
Daniel Loveless	Anti-Tamper IC Forensics and RF-Level DIscrimiNation FOR IMproved Trust (INFORM)	Extreme Environment Technologies	$90,000	$70,149**
Mohamad Mahtabi	Development of Multi-Objectively Optimized Interatomic Potentials for Computational Design of High Temperature Actuator Materials	Advanced Modeling and Simulation	$90,000	$44,812**
Ashley Manning-Berg	Decomposition Modeling of Microbial Mat Ecosystems to Quantify Earth's Early Fossil Record	Health and Biological Systems	$90,000	$25,459**
Hong Qin	Addressing Sampling Biases in Genome-wide Association Study for SARS-CoV-2	Health and Biological Systems	$90,000	$76,143**
Reetesh Ranjan	Modeling of Transition to Turbulence in Large Eddy Simulation using the Two Level Simulation Approach	Advanced Modeling and Simulation	$89,675	$72,588**

*** Due to COVID-19, some or all of the remaining funds on projects marked with asterisks were approved as carryover into FY2023 to support student researchers.*

Schedule 7

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution: UT Chattanooga

Center: Center of Excellence is Applied Computational Science & Engineering

	FY 2021-22 Actual			FY 2022-23 Proposed			FY 2023-24 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries (Exclude Longevity from Salaries and report separately)									
Faculty	$128,191	$238,069	**$366,260**	$166,971	$310,090	**$477,061**	$129,694	$240,861	**$370,556**
Other Professional	$3,102	$5,761	**$8,864**	$4,041	$7,504	**$11,545**	$3,139	$5,829	**$8,968**
Clerical/ Supporting	$6,018	$11,176	**$17,194**	$7,838	$14,557	**$22,396**	$6,088	$11,307	**$17,396**
Assistantships	$90,269	$167,642	**$257,911**	$117,577	$218,357	**$335,934**	$91,328	$169,608	**$260,936**
Total Salaries	**$227,580**	**$422,648**	**$650,228**	**$296,427**	**$550,508**	**$846,936**	**$230,249**	**$427,605**	**$657,855**
Longevity (Excluded from Salaries)	$661	$1,228	**$1,889**	$861	$1,599	**$2,460**	$669	$1,242	**$1,911**
Fringe Benefits	$34,425	$63,931	**$98,356**	$44,839	$83,272	**$128,111**	$34,828	$64,681	**$99,510**
Total Personnel	**$262,666**	**$487,807**	**$750,473**	**$342,127**	**$635,379**	**$977,507**	**$265,746**	**$493,529**	**$759,275**
Non-Personnel									
Travel	$8,169	$15,171	**$23,339**	$10,640	$19,760	**$30,400**	$8,265	$15,349	**$23,613**
Software	$25,811	$47,934	**$73,745**	$33,619	$62,436	**$96,055**	$26,114	$48,497	**$74,610**
Books & Journals			**$0**			**$0**			**$0**
Other Supplies	$18,378	$34,130	**$52,507**	$23,937	$44,455	**$68,392**	$18,593	$34,530	**$53,123**
Equipment	$49,013	$91,025	**$140,038**	$63,841	$118,562	**$182,402**	$49,588	$92,092	**$141,680**
Maintenance	$1,185	$2,200	**$3,385**	$1,543	$2,866	**$4,409**	$1,199	$2,226	**$3,425**
Scholarships	$40,158	$74,579	**$114,737**	$52,307	$97,141	**$149,447**	$40,629	$75,454	**$116,083**
Consultants			**$0**			**$0**			**$0**
Renovation			**$0**			**$0**			**$0**
Other (Specify):			**$0**			**$0**			**$0**
Print	$64	$118	**$182**	$83	$154	**$237**	$64	$119	**$184**
Other Personal Services	$1,913	$3,552	**$5,465**	$2,491	$4,626	**$7,118**	$1,935	$3,594	**$5,529**
Special Commercial Services	$28,792	$53,470	**$82,262**	$37,502	$69,646	**$107,148**	$29,129	$54,097	**$83,227**
Memberships	$25	$46	**$70**	$32	$59	**$91**	$25	$46	**$71**
Student Fees	$12,530	$23,270	**$35,800**	$16,321	$30,310	**$46,630**	$12,677	$23,543	**$36,220**
Group arranged event	$46	$85	**$130**	$59	$110	**$170**	$46	$86	**$132**
Total Non-Personnel	**$186,081**	**$345,579**	**$531,661**	**$242,375**	**$450,124**	**$692,499**	**$188,264**	**$349,633**	**$537,897**
GRAND TOTAL	**$448,747**	**$833,387**	**$1,282,134**	**$584,502**	**$1,085,504**	**$1,670,006**	**$454,010**	**$843,162**	**$1,297,172**
Revenue									
New State Appropriation		$821,517	**$821,517**		$849,116	**$849,116**		$891,572	**$891,572**
Carryover State Appropriation		$335,350	**$335,350**		$323,480	**$323,480**		$0	**$0**
New Matching Funds	$405,600		**$405,600**	$405,600		**$405,600**	$405,600		**$405,600**
Carryover from Previous Matching Funds	$134,957		**$134,957**	$91,810		**$91,810**	$0		**$0**
Total Revenue	**$540,557**	**$1,156,867**	**$1,697,424**	**$497,410**	**$1,172,596**	**$1,670,006**	**$405,600**	**$891,572**	**$1,297,172**
	$91,810	**$323,480**							

Schedule 7

FY2022 PUBLICATIONS AND PRESENTATIONS (of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings

Suggs, E.D. 2019. Meta-textual analysis of biological research. ACM meeting, Gatlinburg, TN.

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

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

Faxon, A., **Hossain, A.**, Mies, J., and Shirmeen, T., 2022, Studying Suspended Sediment Concentrations in the South Chickamauga Creek using Satellite Imagery and Numeric Modeling, ASPRS 2022 Annual Conference, Virtual, March 21-25, 2022.

Faxon, A., **Hossain, A.**, Mies, J., and Shirmeen, T., Studying Suspended Sediment Concentrations in the South Chickamauga Creek of Chattanooga, TN using Satellite Imagery, Digital Image Processing, and Numeric Modeling. NCUR 2022 @Home on April 4-8, 2022.

Hossain, A., and Mathias, C., 2021, Remote Sensing of Water Quality in the Tennessee River Using Sentinel-2 Imagery, GSA Southeastern Section - 70th Annual Meeting – 2021, April 1-2, 2021, Online Meeting. GSA Abstract #362338.

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

Hossain, A., Blanton, R., and Mathias, C., 2019, Surface Water Quality Monitoring Using Remote Sensing Technology in Chattanooga. SWPBA 46th Annual Meeting in Chattanooga, TN October 14th to 17th, 2019.

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

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

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

Hossain, A. and Mathias, C., 2021, Remote Sensing of Water Quality Using Planet Dove Imagery, 6th Annual UTC Research Dialogue, April 12-15, 2021. The University of Tennessee at Chattanooga.

Mathias, C. and **Hossain, A**., 2020, Bathymetric digital elevation model for the Tennessee River. 5th Annual UTC Research Dialogue, April 14-15, 2020. The University of Tennessee at Chattanooga. Conference canceled due to COVID-19 situation.

Hossain, A., Blanton, R., and Mathias, C., 2020, Surface water quality estimation in Southeast Tennessee using Sentinel - 2 satellite imagery. 5th Annual UTC Research Dialogue, April 14-15, 2020. The University of Tennessee at Chattanooga. Conference canceled due to COVID-19 situation.

"A modeling tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." Geological Society of America NC/SE Joint Sectional Meeting, Cincinnati, OH, April 7–8, 2022. (**Stephanie DeVries**)

"A modeling tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." Geological Society of America 2020 Connects Online Meeting, October 27, 2020. (**Stephanie DeVries**)

DeVries, S.L., *Hooten, W. (2020). A C++ tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." Fall Meeting of the American Geophysical Union.

"A C++based model for estimating the concentration of nitrate at a municipal well in central Wisconsin." Presented to the Wisconsin Nitrate Task Force on August 21, 2020. (**Stephanie DeVries**)

DeVries, S.L., *Hooten, W. (2021). A C++ tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." UTC Scholar ReSEARCH Dialogues.

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

Shi, Y., Maya, D., Ratner, A. Predicting Steam-Gasification Output Using Artificial Neural Networks. ASME International Mechanical Engineering Congress and Exposition 2021.

Johnson, G., **Shi, Y**. Prediction of Gasification Outputs via Machine Learning Approaches. National Conference on Undergraduate Research NCUR 2022.

Ward, B., **Shi, Y**. Prediction of Gasification Outputs via Supervised Learning Approaches. National Conference on Undergraduate Research NCUR 2021.

Johnson, G., **Shi, Y**. Prediction of Gasification Outputs via Machine Learning Approaches. UTC College of Engineering Tech Symposium 2022.

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

AMS Sectional Meeting University of California Riverside, November 2019 (**E. Panagiotou**)

Joint Mathematics Meetings, Denver, January 2020 (**E. Panagiotou**)

Topology Seminar, George Washington University, March 2020 (**E. Panagiotou**)

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

Conference on Physical Knotting, Vortices and Surgery in Nature, Novosibirst State University, Russia, July 08 2020 (virtual) (**E. Panagiotou**)

Quantum Entanglement Seminar, Organized by L. H. Kauffman, July 09 2020 (virtual) (**E. Panagiotou**)

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

AMS Sectional Meeting, University of Virginia (*canceled due to COVID19*) (**E. Panagiotou**)

Topology Workshop, Institute of Advance Study, April 2020, UPenn (*canceled due to COVID19*) (**E. Panagiotou**)

SIAM Conference on Mathematical Aspects of Materials Science, May 2020, Bilbao, Spain (*canceled due to COVID19*) (**E. Panagiotou**)

J. Wang, "Immersed boundary and immersed domain methods for fluid-structure interaction", Special Session on Applicable Analysis and Control Theory for Fluid and Fluid-Structure PDEs, SIAM (*canceled due to COVID19*) (**E. Panagiotou**)

Conference on Analysis of Partial Differential Equations, La Quinta, CA, December 2019. (*canceled due to COVID19*) (**E. Panagiotou**)

Y. W. Wang, talk at SERMACS 2019, October 2019 (*canceled due to COVID19*) (**E. Panagiotou**)

Gildernew, Evan and **Panagiotou, E**. The effects of topological entanglement on viscoelastic properties of polymers, poster presentation at UTC Research Dialogues

Software

A. Hossain, J. Bathi plan to develop partnership with commercial satellite companies like Planet Laboratory Inc. to estimate satellite observed water quality data at regular intervals and/or as needed using the developed models.

Nitrate Calculator – A C++ executable program that estimates the annual average nitrate concentration of groundwater in a high-capacity pumping well using a look-up table of nitrate losses from USDA land cover classifications and gridded input data: time-of-travel capture zone, annual recharge depth, land cover. The executable file developed for this project is intended to be an open-access resource with potential use among water resource professionals.The software is downloadable at:

https://github.com/garretthooten/NitrateCalculatorGUI/releases/tag/v1.2.1 (**Stephanie DeVries**)

Refereed Publications

Olivier, C. A., Jaeggi, A. V., **Hayes, L. D.**, & Schradin, C. (2022). Revisiting the components of Macroscelidea social systems: Evidence for variable social organization, including pair-living, but not for a monogamous mating system. Ethology, 128(5), 383-394.

Hossain, A. Mathias, C. and Blanton, R., 2021, Remote Sensing of Turbidity in the Tennessee River Using Landsat 8 Satellite, Remote Sensing, 2021, 13, 3785. https://doi.org/10.3390/rs13183785.

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

Dey, P., Roy, S., **Bathi, J.**, Mishra, A., Leasi, F., and **Hossain, A.**, 2021, Parameter Sensitivity Analysis of the HSPF Model on a Pervious Landcover Dominated Watershed, Proceedings of EWRI Congress 2021, 561-574, https://ascelibrary.org/doi/abs/10.1061/9780784483466.051.

Hossain, A., Mathias, C., and Blanton, R., Exploring the potential of Sentinel - 2 satellite imagery for quantitative surface water quality estimation in Southeast Tennessee. The manuscript is under preparation and to be submitted to Remote Sensing of the Environment. (In preparation)

Hossain, A., Blanton, R., and Mathias, C., Quantitative Remote Sensing of Surface Water Quality in Southeast Tennessee Utilizing Planet Dove Imagery. The manuscript is under preparation and to be submitted to Remote Sensing. (In preparation)

DeVries, S., *Hooten, W.G., *Mollica, M. “A model for estimating nitrate in high-capacity wells as function of land use and time-of-travel capture zones in well-oxygenated sand and gravel aquifers.” – Pending submission to Environmental Software & Modeling (Impact Factor 4.807).

DeVries, S., Bradbury, K., and Cardiff, M. (2022). “A Groundwater Flow Model for Waupaca, WI.” Wisconsin Geological Survey and Natural History Survey Technical Report. 007, 88 p., https://doi.org/10.54915/xdis1726.

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

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

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

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

Invention Disclosures

We are aware of invention disclosures from Sungwoo Yang, Hamdy Ibrahim, and David Giles, all of whom are recent CEACSE awardees.

Patent Applications

None during this reporting period.

EXTERNAL FUNDING

Yunye Shi, Lead PI

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

Project Title: Predicting Biomass Gasification Output – A Machine Learning Approach

Proposal Submissions

- Impact of Additives on Combustion of Bio-derived Fuels. Agency: NSF ERI. Duration: 09/2023-07/2025. Total amount: $199,523. Role: Principal Investigator. Submission in preparation.
- Impact of Additives on Combustion of Bio-derived Fuels. Agency: NSF ERI. Duration: 09/2022-07/2024. Total amount: $199,523. Role: Principal Investigator. Not funded.
- Impact of Additives on Combustion of Bio-derived Fuels. Agency: DOE ORAU Ralph E. Powe Junior Faculty Enhancement Awards. Total amount: $5,000. Role: Principal Investigator. Not funded.

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

- NSF grant webinars
- College grant writing workshops

Azad Hossain, Lead PI

Co-PI(s): Jejal Bathi, Mark Schorr
Other Personnel: Richard Blanton, Graduate Research Assistant, Caleb Mathias - Undergraduate Research Assistant, Connor Firat - Graduate Research Assistant, Shuvashish Roy - Graduate Research Assistant, and Syed Tareq - Graduate Research Assistant

Project Title: Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies

Proposal Submissions

- Urban Streams Restoration Project. Agency: Tennessee Wildlife Resources Agency. Duration: 07/01/2020–06/30/2023. Amount: $36,000. Role: Co-Principal Investigator (Principal Investigator: Mark Schorr).

Contracts/Awards Received

- Urban Streams Restoration Project: Measuring the Efficacy of Habitat Mitigation/Restoration Efforts on Chattanooga Area Streams: Citico Creek, Friar Branch, and Mountain Creek. Agency: city of Chattanooga. Duration: 01/01/2020-08/31/2022. Amount: $43,869. Role: Co-Principal Investigator (Principal Investigator: Mark Schorr). Pending.
- Integration of Remote Sensing Technology with Hydrodynamic Models for Surface Water Quality Monitoring in Southeast Tennessee. Agency: USGS through Tennessee

Water Resources Research Center (TNWRRC). Duration: March 1, 2020-February 28, 2021. Total amount: $24,976 (Federal) and $50,390 (Non-federal). Role: Principal Investigator. Not funded.

- Integration of remote sensing technology and numerical model for water quality study in Mississippi Sound. Agency: The Mississippi Based RESTORE Act Center of Excellence (MBRACE) at the University of Southern Mississippi. Duration: 01/01/2020-12/31/2021. Total amount: $87, 88. This proposal was submitted by The University of Mississippi in collaboration with The University of Tennessee at Chattanooga (UTC). Role: Co-Principal Investigator [UTC Principal Investigator]. Not Funded.

Sponsored Program Capacity Building Activities

Attended webinar organized by the Tennessee Water Resources Research Center (TNWRRC) at the University of Tennessee at Knoxville after getting invited to submit a proposal to the National Institutes for Water Resources at the U. S. Geological Survey.

Hamdy Ibrahim, Lead PI

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

Project Title: Corrosion Modeling of Magnesium-based Fixation Hardware for Mandibular Reconstruction Surgeries

Proposal Submissions

- Ibrahim, H., “Treating Bone Trauma Using ResorbFix”, I-Corps Teams, submitted to the National Science Foundation (NSF), 2020. Requested amount: $50,000. Status: Awarded.
- Ibrahim, H., Mahtabi, M., Danquah, M., Elliot, T., Palchoudhury, S., Elliot, L. & Panagiotou, E. “Acquisition of a customized metal additive manufacturing system for multidisciplinary research activities”, Major Research Instrumentation Program: (MRI), submitted to the National Science Foundation (NSF), 2020. Requested amount: $261,500. Status: Not Funded.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Loren Hayes Lead PI

Co-PI(s): Jin Wang
Other Personnel: Craig Tanis (former co-PI), Elizabeth Pope (student), Evan Suggs (student), Braxton Anzalone (student), Azad Hossain (unfunded faculty)

Project Title: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models

Proposal Submissions

- NSF IOS, Comparative and computational analyses of climatic and life history drivers of variable social organization in mammals. Submitted in summer 2020, declined. (Hayes, Tanis, and Wang co-PIs)

Contracts/Awards Received

- N/A

Sponsored Program Capacity Building Activities

- Consultations with NSF IRES program officer.
- Managed my NSF IRES grant.

Mina Sartipi, Lead PI

Co-PI(s): Farah Kandah, Osama Osman
Other Personnel: N/A

Project Title: Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications

Proposal Submissions

- A research statement was submitted to the Tennessee Department of Transportation that builds on the integrated platform being developed in this project.

Contracts/Awards Received

- N/A

Stephanie DeVries, Lead PI

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

Project Title: A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers

Proposal Submissions

No proposals related to this CEACSE award have yet been submitted.

Contracts/Awards Received

None to report.

Sponsored Program Capacity Building Activities

None to report.

Eleni Panagiotou, Lead PI

Co-PI(s): Jin Wang, Abi Arabshahi, W. Y. Yang, Chris Dowell
Other Personnel: Evan Gildernew, Jarod Wright, Philip Smith, Dahlen Elstran

Project Title: A study on the local and global effects of polymer entanglement in material properties and biological functions

Proposal Submissions

- NSF Proposal on Entanglement in Polymers submitted prior to reporting period but immediately related to the proposed work.
- NSF CAREER: Topology of the active polymers (awarded)
- NSF MODULUS (not funded)
- ORAU Powe award (not funded)

Contracts/Awards Received

- NSF Proposal on Entanglement in Polymers, DMS Computational Mathematics, $125,000.
- NSF CAREER award: DMR and DMS, $537,000

Sponsored Program Capacity Building Activities

- Visited NSF to serve as reviwer. During that visit, I had planned meetings with two program officers in DMS Computational Mathematics and DMS Math Biology
- Attended an NSF meeting at JMM meeting Denver
- Attended workshops held from ORSP for preparing NSF CAREER proposals
- Organized BIRS meeting, 2021

OVERVIEW OF FY2023 PROJECTS

The following awardees and projects, selected for funding in February 2022, 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: Synthesis of Novel Aerogels for use in Retrofit Window Treatments which are Inexpensively Manufactured, Maintain Transparency Standards, and Dramatically Reduce Heat Loss
Investigator: Sungwoo Yang
Thrust: Health & Biological Systems + Extreme Environment Technologies
Amount: $89,675

Abstract: 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.

Title: Modelling Archaeo-Acoustic Phenomena as a Means of Developing a Method for Non-Invasive, Remote Detection of Underwater Archaeological Sites
Investigators: Morgan Smith, Boris Belinskiy
Thrust: Environmental Sustainability and Climate Systems + Advanced Modeling and Simulation
Amount: $99,938

Abstract: 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.

Title: Study of Differential Diffusion Effects in Stratified Turbulent Flows using a Hybrid Multi-Scale Modeling Strategy
Investigators: Reetesh Ranjan
Thrust: Advanced Modeling & Simulation
Amount: $93,867

Abstract: 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.

Title: Integrating Google Trends Analytics into Geographically Weighted Model of Vaccine Hesitancy
Investigators: Lani Gao, Nagwan Zahry and Ziwei Ma
Thrust: Health and Biological Systems + Advanced Modeling and Simulation
Amount: $95,577

Abstract: 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

Title: Exploring entanglements in polymer network topologies with single-chain nanoparticles
Investigators: Meredith Barbee, Eleni Panagiotou
Thrust: Advanced Modeling & Simulation + Health and Biological Systems
Amount: $100,000

Abstract: The proposed research is focused on two main goals: (1) quantifying the effect of entanglements in polymer networks on the mechanical properties of the material and (2) developing design principles for an unexplored network topology in hydrogel materials based on the unfolding of single-chain polymer nanoparticles. Through a combination of simulations and characterization of synthetic materials, we hope to uncover fundamental relationships important in designing polymer networks and establish a framework for developing hydrogels that are highly extensible, overcoming limitations to the use in these typically brittle materials.

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 FY2022.

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 FY2022 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.

Appendix A
Faculty Biosketches

NAME: Yunye Shi

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)
Huazhong University of Science and Technology	Wuhan, China	Power & Energy Engineering	B.S.	2008
Huazhong University of Science and Technology	Wuhan, China	Power & Energy Engineering	M.S.	2010
The University of Iowa	Iowa City, IA	Mechanical Engineering	PH.D.	2016

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

From - To	Position Title, Organization and Location
08/2020-till date	Assistant Professor, The University of Tennessee at Chattanooga
08/2015-07/2020	Assistant Professor, St. Ambrose University

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

1. Powell, K.*, Shi, Y. Gasification Based Waste Tire Integrated Energy Conversion Systems. 2022ASEE Southeast Conference.
2. Johnson, Greg.*, Shi, Y. Prediction of gasification outputs via machine learning approaches. 2022NCUR. April 2022.
3. Marques, T., Santiago, Y., Maya, D., Shi, Y. Environmental and energetic evaluation of refuse-derived fuel gasification for electricity generation. Processes. 2021.
4. Shi, Y., Maya, D., Ratner, A. Predicting Steam-Gasification Output Using Artificial Neural Networks. ASME 2021 International Mechanical Engineering Congress and Exposition. 2021.
5. Zang, G., Jia, J., Shi, Y., Sharma, T., Ratner, A. Modeling and economic analysis of waste tire gasifi-cation in fluidized and fix bed gasifiers. Waste Management. 2019.

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

6. Shi, Y., Maya, D., Nascimento, R., Sharma, T., Ratner, and A., Lora, E. Experimental and simulation studies of corn kernel gasification in a double air stage downdraft reactor. ASME 2018International Mechanical Engineering Congress and Exposition. 2018.
7. Prosise, J. K., Romatoski, R., Shi, Y, Stonedahl, S. H. Inspiring girls to pursue STEM (ages three to thirteen): a recipe for a successful outreach event. American Society for Engineering Education2018 Conference Proceedings, 2018.
8. Chen, C., Liu, Y., Greig, J., Shen, Z., Shi, Y. The Impacts of COVID-19 on Clean Energy Labor Markets: Evidence from Multifaceted Analysis of Public Health Interventions and COVID-health Factors. Energy Policy. 2021.
9. Sharma, T., Maya, D., Nascimento, R., Shi, Y., Ratner, A., Lora, E., Mendes, L., Palacios, J., Andradei, R., 2018. An Experimental and theoretical study of the gasification of miscanthus briquettes in a double-stage downdraft gasifier: syngas, tar and biochar characterization. Energies.

10. Huang, X., Wang, D., Shi, Y., Liu, Z., Zheng, C., Conversion of char Nitrogen to NO in O2/CO2 environment. Journal of Engineering Thermophysics. Journal of Engineering Thermophysics. 2010.

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

(i) Topic organizer for combustion mini-symposium session "bioenergy and biofuel", ASME International Mechanical Engineering Congress, 2018 and 2019.
(ii) Reviewer for ASME International Mechanical Engineering Congress, 2018-2021.
(iii) IMECE Combustion mini-Symposium topic organizer, 2018-2019
(iv) Reviewer for Fuel, Journal of BioResources, International Journal of Energy Research, and Flow, Turbulence and Combustion, Journal of the Energy Institute
(v) Guest editor of a special issue on Gasification Processing of Biomass and Refuse Derived Fuel of Processes, 2021

NAME: Azad Hossain

POSITION TITLE & INSTITUTION: Associate 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)
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
(see PAPPG Chapter II.C.2.f.(i)(b))

From - To	Position Title, Organization and Location
Aug. 2022-Present	Associate Professor, Department of Biology, Geology and Environmental Science The University of Tennessee at Chattanooga
Aug. 2016- July 2022	Assistant Professor, Department of Biology, Geology and Environmental Science The University of Tennessee at Chattanooga
July 215 – July 2016	Visiting Assistant Professor, Department of Geology and Geological Engineering The University of Mississippi
Sept. 2011–June 2015	Research Scientist, National Center for Computational Hydroscience and Engineering The University of Mississippi
Dec. 2010 – June 2015	Adjunct Assistant Professor, Department of Geology and Geological Engineering The University of Mississippi
Aug. 2008 – Sept. 2011	Post Doct. Res. Associate, National Center for Computational Hydroscience and Engineering The University of Mississippi
Mar. 2007 – Aug. 2008	Geographic Information Systems Technician The University of Mississippi Geoinformatics Center
May 1999 – Dec. 2001	Remote Sensing and GIS Analyst Center for Environmental and Geographic Information Services. Dhaka, Bangladesh.

C. PRODUCTS

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

Products Most Closely Related to the Proposed Project

1. Hossain, A. Mathias, C. and Blanton, R., 2021, Remote Sensing of Turbidity in the Tennessee River Using a Landsat 8 Satellite, Remote Sensing, 2021, 13, 3785. https://doi.org/10.3390/rs13183785.
2. Hossain, A., Stuart, W., Mies, J., and Brock-Hon, A., 2021, Investigating Urban Heat Island (UHI) Impact for the City of Chattanooga, Tennessee Using GIS and Remote Sensing, in "Handbook of Climate Change Mitigation and Adaptation", Maximilian Lackner MBA. (editor), Springer International Publishing.
3. Hossain, A. and Greg Easson, 2022, 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.
4. Hall, J. and Hossain, A., 2020, Mapping Urbanization and Evaluating Its Possible Impacts on Stream Water Quality in Chattanooga, Tennessee, Using GIS and Remote Sensing. Sustainability, 12 (5), 1980, 1-46.
5. Hossain, A., 2013, Flood Inundation and Crop Damage Mapping: A Method for Modeling the Impact on Rural Income and Migration in Humid Deltas, in 'Climate Vulnerability: Understanding and Addressing Threats to Essential Resources' Faisal Hossain (volume editor), Roger Pielke Sr. (series editor), Vol. 5. pp. 357-374, Elsevier Inc., Academic Press, ISBN: 9780123847034.
6. Hossain, A., 2019, Investigating Urban Heat Island (UHI) Impact for the City of Chattanooga, TN Using GIS and Remote Sensing, ASPRS Annual Conference 2019, Denver, CO, January 28-31, 2019.

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

1. Chao, X., Jia, Y., Hossain, A., and Zhang, Y., 2021, Numerical Simulation of Sediment Transport, Phytoplankton Biomass and Salinity Recovery Processes in Lake Pontchartrain due to Bonnet Carré Spillway Flood Release, Ecological Engineering, 160 (2021) 106151.
2. Blanton, R. and Hossain, A., 2020, Mapping the Recovery Process of Vegetation Growth in the Copper Basin, Tennessee Using Remote Sensing Technology. GeoHazards, 1, 31-43.
3. Hossain, A., and Easson, G., 2016, Soil Moisture Estimation in South-eastern New Mexico Using High Resolution Synthetic Aperture Radar (SAR) Data, Geosciences, 6(1), pp. 1-20.

D. SYNERGISTIC ACTIVITIES

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

1. Taught both undergraduate and graduate courses on GIS, remote sensing, and spatial analysis. Also taught undergraduate course on physical geology, historical geology, and environmental geology.
2. Served/Serving as a primary advisor/committee member/mentor of graduate and undergraduate students.
3. Served/Serving in different departmental and university committees.
4. Served/Serving as PI/Co-PI for internal and external research grants
5. Reviewed different journal articles and external grants.
6. Serving on journal review and editorial board
7. Served as conference moderators and organized/helped in organizing research workshops.

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

A. Professional Preparation:

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

Appointments:

2021 – Present	Professor of Practice University of Tennessee at Chattanooga, TN
2017 – 2021	Visiting Assistant Professor University of Tennessee at Chattanooga, TN
20017 – Present	Principal Engineer Syntec Consultants, LLC, TN
2009 – 2016	Principal Civil Engineer Global Systems International, LLC, AL
20014 – 2015	Research Scientist Jackson State University, MS
2013 – 2015	Adjunct Faculty Jackson State University, MS
2006 - 2008	Graduate Research Assistant NSF ALEPSCoR Center for Optical Sensors and Spectroscopies, University of Alabama

Representative Publications:

1. Bathi, J. R., Wright, L., Khan, E. Critical Review of Engineered Nanoparticles: Environmental Concentrations and Toxicity. Current Pollution Reports. 1-21. 10.1007/s40726-022-00237-4, 2022.
2. Bathi, J. R., Roy, S., Tareq, S.M., Potts, G. E., Palchoudhury, S., Sweck, S., Gadhamshetty, V. Dispersion and Aggregation Fate of Individual and Co-Existing Metal Nanoparticles under Environmental Aqueous Suspension Conditions. Materials. 15. 6733. 10.3390/ma15196733, (2022).
3. Tareq, S.M., Boutchuen, A., Roy, S., Jur G., Bathi J.R., Palchoudhury S. A Dynamic Light Scattering Approach for Detection of Nanomaterials in Tennessee River", Water Resources Research, vol. 57, no. 8, 2021.doi: 10.102912020WR028687.
4. Harvey., C., Neidich., B., Ellis., R., Gomez., D. O., Belton., A and Bathi., J.R. "Retrofit Upgrade of Stormwater Controls with Real-Time Mechanism for Smart and Sustainable Urban Water Resources Management," 2021 Waste-management Education Research Conference (WERC), 2021, pp. 1-9, DOI: 10.1109/WERC52047.2021.9477537.
5. Dey., P., Roy., S., Bathi., J.R., Mishra.,M., Leasi., F., Azad Hossain., A.K.M. Parameter Sensitivity Analysis of the HSPF Model on a Pervious Landcover Dominated Watershed. ASCE World Environmental and Water Resources Congress 2021 : Planning a Resilient Future along America's Freshwaters, 2021.
6. Bathi, J.R., Moazeni, F., Upadhyayula, V.K.K., Chowdhury, I. Palchoudhury, S., Potts, G. E., Gadhamshetty, V. Behavior of engineered nanoparticles in aquatic environmental samples: Current status and challenges, Science of The Total Environment, Volume 793, 2021,148560, ISSN 0048697, https://doi.org/10.1016lj.scitotenv.202l .148560.

7. Bathi, J.R., and H.S. Das., "Vulnerability of Coastal Communities from Storm Surge and Flood Disasters," International Journal of Environmental Research and Public Health, Vol. 13, pp 239, 2016.
8. Eppakayala, V.J., Bathi, J. R., R. Pitt, S. E. Clark. "Stormwater Treatment at an Industrial Site using a Dry Infiltration Pond with Pre-Treatment". International Low Impact Development Conference 2015, Houston, TX, January 19 – 21, 2015.
9. Pitt, R., K. Goodson, O. Ogburn, V. Eppakayala, Bathi, J.R., Wilson, B., Subramaniam, S., and Clark, S., "Identification and Treatment of Emerging Contaminants in Wet Weather Flows," EPA Contract: EP-C-07-014. Office of Research, EPA, 2013. (Research Report)
10. Bathi, J. R., R. Samual. "Introduction to Changing Site Design Standards for Stormwater Management." Annual Mississippi Water Resources Conference, Jackson, MS, April 2-3, 2013.
11. Bathi, J. R., R.E. Pitt, and S.E. Clark., "Polycyclic aromatic hydrocarbons in urban stream sediments," Advances in Civil Engineering, 2012.
12. Peters, R, W., P, Sharma, J. R. Bathi. "Benchmarking the Integration of Sustainability into Engineering Curricula at US Institutions of Higher Education" AIChE Annual Meeting San Francisco, CA, 2006.

Synergistic Activities:

1. Environmental Engineering Program Coordinator, Civil and Chemical Engineering, University of Tennessee at Chattanooga, TN 2021 - Present
2. Board member of the Diffuse Pollution and Eutrophication Specialist Group with the International Water Association (IWA), 2022 - present
3. Secretory, Water Pollution Engineering Committee, Environmental and Water Resources Institute of the American Society of Civil Engineers, 2022 -Present.
4. Reviewer, U.S. Environmental Protection Agency (EPA) Science to Achieve Results (STAR) Fellowship Program, 2015
5. Member, Urban Watershed Management Committee, Environmental and Water Resources Institute of the American Society of Civil Engineers, 2009
6. Member, Students and Young Professional Committee, Water Environment Federation (WEF), 2007 – 2015
7. Founding Member, Secretary/Treasurer of Black Warrior Environmental Association (BWEA), Student chapter of Alabama Water Environmental Federation and WEF, 2007 – 2008

Mark Steven Schorr
Professor
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The University of Tennessee at Chattanooga
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(a) Professional Preparation

Southeastern Louisiana University, LA	Zoology	B.S.	1985
Mississippi State University, MS	Zoology	M.S.	1988
Mississippi State University, MS	Forest Resources (Fisheries Management)	Ph.D.	1994
Mississippi State University, MS	Post-doctoral Fellow at the Department of Wildlife and Fisheries		1991-1993
University of Oklahoma, OK	Post-doctoral Fellow at the Biological Station		1993-1994

(b) Appointments

2004 - Present	Professor Department of Biology, Geology & Environmental Science University of Tennessee at Chattanooga, TN
1999 - 2004	Associate Professor Department of Biology, Geology & Environmental Science University of Tennessee at Chattanooga, TN
1994 - 1999	Assistant Professor Department of Biology, Geology & Environmental Science University of Tennessee at Chattanooga, TN

(c) Products

(i) Five products most closely related to the proposed project

Schorr, M.S. and T. Wilson. 2006. Assessments of water quality, habitat, and aquatic macrofauna in a Cumberland Plateau stream: a geographic information system (GIS) approach. Final Report for the Southern Appalachian Information Node (SAIN) of the National Biological Information Infrastructure (NBII) program.

Schorr, M.S., E. Crews, P. Freeman, J. Long, P. Johnson, and D. Fritz. (2001). Assessment of water quality and aquatic macrofauna in Chattanooga area streams. Contract No. R04101154-64. Final Report. City of Chattanooga, Department of Public Works, Stormwater Management Section, Chattanooga, Tennessee, 444 pp.

Schorr, M.S., C.H. Nelson, and G. Van Horn. (1997). Ecological assessment of streams impacted by acid mine drainage in the North Chickamauga Creek System, Tennessee, and an evaluation of the mitigation potential of constructed wetlands. Contract Number ID-6-05876-6-00. Annual Report. Tennessee Wildlife Resources Agency, Nashville, Tennessee, 72 pp.

Long, J.* and M.S. Schorr. (2005). Effects of watershed urban land use on environmental conditions and fish assemblages in Chattanooga area streams (Tennessee-Georgia). Journal of Freshwater Ecology 20:527-537.

Freeman, P.* and M.S. Schorr. (2004). Influence of watershed urbanization on fine sediment and macroinvertebrate assemblage characteristics in Tennessee Ridge and Valley streams. Journal of Freshwater Ecology 19:353-362.

(ii) Five other significant products

Wolfe D.N., Schorr M, Hanson M, Nelson CH, Richards SM. (2015). Hazard assessment for a pharmaceutical mixture detected in the upper Tennessee River using *Daphnia magna*. Global Journal of Environmental Science and Management 1(1):1-14

Shaw J, Shafer H.L., Leonard OR, Kovach MJ, Schorr M, Morris AB. (2014). Chloroplast DNA sequence utility for the lowest phylogenetic and phylogeographic inferences in angiosperms: the tortoise and the hare IV. American Journal of Botany 101(11):1-1.

Schorr M.S., Dyson M.C., Nelson C.H., Van Horn G.S., Collins D.E., Richards S.M. (2013). Effects of stream acidification on lotic salamander assemblages in a coal-mined watershed in the Cumberland Plateau. Journal of Freshwater Ecology, DOI:10.1080/02705060.2013.778219.

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

Schorr, M.S. and J.C. Baker. (2006). Localized effects of coal mine drainage on fish assemblages in a Cumberland Plateau stream in Tennessee. Journal of Freshwater Ecology 21:17-24.

(d) Synergistic Activities

Selected Research Grants (External Funding)
Schorr MS (PI) (2012). Post-stream restoration assessments for Citico Creek and Friar Branch. City of Chattanooga, Department of Public Works, Stormwater Management, $42,079.

Schorr, MS (PI), Wilson TP (2005-2006). Assessments of water quality, habitat, and aquatic macrofauna in a Cumberland Plateau stream: a geographic information system (GIS) approach. National Biological Information Infrastructure - Southern Appalachian Information Node (This project was a component of a larger project, "University of Tennessee Core Tasks for the NBII SAIN Node"; principal investigators: H. Spratt, G. Litchford, D. Aborn, T. Wilson, and M. Schorr total budget: $132,545.

Schorr MS (PI), Nelson CH, Fritz D, Johnson P (1997-2000). Investigation of the effects of watershed land use on water quality and aquatic biota in urban streams in Chattanooga, Tennessee. City of Chattanooga, Department of Public Works, Stormwater Management Section, $150,300 (four grants).

Schorr MS (PI), Nelson CH, Van Horn G (1997). Evaluation of the adequacy of constructed wetlands to improve limnological conditions and restore native fish assemblages in streams impacted by acid mine drainage in the North Chickamauga Creek watershed, Tennessee. Tennessee Wildlife Resources Agency, $17,000.

Schorr MS (PI), Nelson CH, Van Horn G (1997). Evaluation of the adequacy of constructed wetlands to improve limnological conditions and native fish assemblages in streams impacted by acid mine drainage in the North Chickamauga Creek Watershed, Tennessee. National Fish and Wildlife Foundation, Washington, D.C., $12,000.

Hamdy Ibrahim
University of Tennessee at Chattanooga (UTC)
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(a) Professional Preparation

Cairo University	Cairo, Egypt	Mechanical Engineering	B.S. 2008
Cairo University	Cairo, Egypt	Mechanical Engineering	M.S. 2012
The University of Toledo	Toledo, OH	Mechanical Engineering	Ph.D. 2017
The University of Toledo	Toledo, OH	Mechanical Engineering	2017-18 (Postdoc)

(b) Appointments

August 2018–present, Assistant Professor, Department of Mechanical Engineering, UTC
Feb. 2018–July 2018, Chief Research Officer, Thermomorph LLC, Toledo, OH

(c) Publications (h-index: 9)

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

- **Ibrahim, H**., Jahadakbar, A., Dehghan, A., Moghaddam, N. S., Amerinatanzi, A., & Elahinia, M. (2018). *In Vitro Corrosion Assessment of Additively Manufactured Porous NiTi Structures for Bone Fixation Applications*. Metals, 8(3), 164.
- Moghaddam, N. S., Saghaian, S. E., Amerinatanzi, A., **Ibrahim, H.**, Li, P., Toker, G. P., Karaca, H. E., & Elahinia, M. (2018). *Anisotropic tensile and actuation properties of NiTi fabricated with selective laser melting*. Materials Science and Engineering: A, 724, 220-230.
- Ma, C., Andani, M. T., Qin, H., Moghaddam, N. S., **Ibrahim, H.**, Jahadakbar, A., Amerinatanzi, A., Ren, Z., Zhang, H., Doll, G.L., & Dong, Y. (2017). *Improving surface finish and wear resistance of additive manufactured nickel-titanium by ultrasonic nano-crystal surface modification*. Journal of Materials Processing Technology, 249, 433-440.
- **Ibrahim, H.**, Klarner, A. D., Poorganji, B., Dean, D., Luo, A. A., & Elahinia, M. (2017). *Microstructural, mechanical and corrosion characteristics of heat-treated Mg-1.2 Zn-0.5 Ca (wt%) alloy for use as resorbable bone fixation material*. Journal of the mechanical behavior of biomedical materials, 69, 203-212.
- **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.

(ii) Five other significant publications:

- **Ibrahim, H**., Luo, A., Dean, D., & Elahinia, M. (2019). *Effect of Zn content and aging temperature on the in-vitro properties of heat-treated and Ca/P ceramic-coated Mg-0.5% Ca-x% Zn alloys*. Materials Science and Engineering: C, 103, 109700.
- **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.**, Mehanny, S., Darwish, L., & Farag, M. (2018). *A comparative study on the mechanical and biodegradation characteristics of starch-based composites reinforced with different lignocellulosic fibers*. Journal of Polymers and the Environment, 26(6), 2434-2447.
- Mehanny, S., Darwish, L., **Ibrahim, H.**, El-Wakad, M. T., & Farag, M. (2016). *High-content lignocellulosic fibers reinforcing starch-based biodegradable composites: properties and applications*. Composites from Renewable and Sustainable Materials, 45.
- **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.

(d) Patents

- **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.

(e) Synergistic Activities

- **Co-organizer** for a symposium on "Advanced Manufacturing, Processing, Characterization, and Modeling of Functional Materials" in the Materials Science & Technology Conference (MS&T 18), Columbus, OH.
- **Guest editor** for Special Issue titled "Engineering Bone-Implant Materials" in the MDPI – Bioengineering Journal.
- **Peer reviewer** for several journals, including for esteemed periodicals *Corrosion Science*, *Journal of Polymers and the Environment*, *Journal of Alloys and Compounds*, *and Sensors & Actuators*: *A*.
- Mentored 7 undergraduate students in senior year research projects and 4 graduate students through their master's thesis projects.
- Participated in the development of a clot removal device "QuickFlow PE" during his employment at the start-up company "Thermomorph". The National Science Foundation (NSF), through its Division of Industrial Innovation & Partnership, awarded Thermomorph's team $50,000 for the development and commercialization of QuickFlow PE, and then awarded Thermomorph $225,000 for further advancing QuickFlow PE in the commercial realm. Dr. Ibrahim's device "QuickFlow" won first prize at the University of Toledo's College of Business and Innovation for the $10,000 Business Innovation Competition.

NAME: Mohammad Mahtabi

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)
University of Tehran	Tehran, Iran	Engineering/ Civil	B.SC	2005
Iran Univ. of Sci. & Tech.	Tehran, Iran	Engineering/ Civil	M.Sc	2008
Mississippi State Univ.	MS, USA	Engineering/ Mechanical	PhD	2017
University of Toledo	OH, USA	Additive Manufacturing, Shape Memory Alloys, Fatigue and Fracture	Postdoc	2017

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

From - To	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

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

Products Most Closely Related to the Proposed Project

- Yadollahi, A., Mahtabi, M. J., Khalili, A., Doude, H. R., and Newman Jr, J. C., Fatigue life prediction of additively manufactured material: Effects of surface roughness, defect size, and shape, Fatigue & Fracture of Engineering Materials & Structures 41.7 (2018): 1602-1614. doi:10.1111/ffe.12799
- Nematollahi, M., Toker, G., Saghaian, S. E., Salazar, J., Mahtabi, M., Benafan, O., ... & Elahinia, M. (2019). Additive manufacturing of ni-rich nitihf 20: Manufacturability, composition, density, and transformation behavior. Shape Memory and Superelasticity, 5(1), 113-124.
- Aboutaleb A., Mahtabi M.J., Bian L., Tschopp M.A., Multi-Objective Accelerated Process Optimization of Mechanical Properties in Laser-based Additive Manufacturing: Case Study on Selective Laser Melting (SLM) Ti-6Al-4V, Journal of Manufacturing Processes 38 (2019): 432-444. doi: 10.1016/j.jmapro.2018.12.040.
- 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.
- Nematollahi M., Jahadakbar A., Mahtabi M.J., Elahinia M., "Additive Manufacturing", 2019, in: Niinomi M. "Metals for Biomedical Devices- 2nd Edition" Woodhead Publishing, Paperback ISBN: 9780081026663

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

- Mahtabi M.J. and Shamsaei N., Fatigue modeling for superelastic NiTi considering cyclic deformation and load ratio effects, Shape Memory and Superelasticity 3 (2017): 250-263. doi: 10.1007/s40830-017-0115-2.
-Ataollahi, S., & 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, 29, 102859.
- Bayati, Parisa, et al., Toward understanding the effect of remelting on the additively manufactured NiTi., The International Journal of Advanced Manufacturing Technology (2020): 1-14.
- Bagheri, A., Mahtabi, M.J. and Shamsaei, N., Fatigue behavior and cyclic deformation of additive manufactured NiTi. Journal of Materials Processing Technology, 252 (2018): 440-453.
-Bagheri, A., Yadollahi, A., Mahtabi, M. J., Paudel, Y., Vance, E., Shamsaei, N., & Horstemeyer, M. F. (2022). Microstructure-Based MultiStage Fatigue Modeling of NiTi Alloy Fabricated via Direct Energy Deposition (DED).

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

(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" in the MDPI . (4) He is a memeber 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.

BIOSKETCH FOR LOREN D. HAYES

A. Professional preparation

Bates College (Maine) Biology B.S. (1992-1996)
Michigan State University Zoology M.S. (1996-1999)
Miami University (Ohio) Zoology Ph.D. (2000-2004)

B. Appointments

2021-present	Full Professor	University of Tennessee at Chattanooga
2014-2020	Associate Professor	University of Tennessee at Chattanooga
2015	Visiting Scholar	USIAS, Strasbourg, France
2012-2014	Assistant Professor	University of Tennessee at Chattanooga
2010-2011	Associate Professor	University of Louisiana at Monroe
2007-2009	Visiting Professor	Universidad Austral de Chile
2004-2010	Associate Researcher P.	Universidad Católica de Chile
2004-2010	Assistant Professor	University of Louisiana at Monroe

C. Products

(i) Five products most closely related to the proposed project (=student)*

(1) Miles, M. I.*, Jaeggi, A. V., Festa-Bianchet, M., Schradin, C., & Hayes, L. D. 2019. Intraspecific variation in Artiodactyla social organisation: A Bayesian phylogenetic multilevel analysis of detailed population-level data. BioRxiv, 603399.

(2) Agnani, P.*, Kauffmann, C., Hayes, L. D., & Schradin, C. 2018. Intra-specific variation in social organization of Strepsirrhines. American Journal of Primatology, 80(5), e22758.

(3) Schradin, C., Hayes, L. D., Pillay, N., & Bertelsmeier, C. 2018. The evolution of intraspecific variation in social organization. Ethology, 124(8), 527-536.

(4) Valomy, M.*, Hayes, L. D., & Schradin, C. 2015. Social organization in Eulipotyphla: evidence for a social shrew. Biology letters, 11(11), 20150825.

(5) Ebensperger, L.A., Villegas, A., Abades, S., & Hayes, L.D. 2014. Mean but not variance in ecological conditions modulate fitness effects of group-living and communal rearing. Behavioral Ecology, 25, 862-870. doi: 10.1093/beheco/aru061

(ii) Five other products (*=student)

(6) Davis, G.,* Vasquez, R., Poulin, E., Oda, E., Bazan- León, E.A., Ebensperger, L.A., & Hayes, L.D. 2016. Octodon degus kin and social structure. Journal of Mammalogy, 97, 361-372.

(7) Wey, T.*, Burger, J.R*., Ebensperger, L.A. & Hayes, L.D. 2013. Reproductive correlates of social network variation in plural breeding degus (*Octodon degus*). Animal Behaviour, 85, 1407-1414.

(8) Hayes, L. D., Chesh, A. S.*, Castro, R. A., Tolhuysen, L. O., Burger, J. R.*, Bhattacharjee, J., & Ebensperger, L. A. 2009. Fitness consequences of group living in the degu *Octodon degus*, a plural breeder rodent with communal care. Animal Behaviour, 78(1), 131-139.

(9) Hofmann, H.A., Beery, A.K., Blumstein, D.T., Couzin, I.D., Earley, R.L, Hayes, L.D., Hurd,

P.L., Lacey, E.A., Phelps, S., Solomon, N.G., Taborsky, M., Young, L.J., & Rubenstein, D.R. 2015. An evolutionary framework for studying mechanisms of social behavior. Trends in Ecology & Evolution, 29, 581-589.
(10) Hayes, L. D., Correa, L. A., Abades, S., Gao, C. L., & Ebensperger, L. A. 2018. Male group members are costly to plurally breeding *Octodon degus* females. Behaviour, 1(aop), 1-36.

D. Synergistic activities
(1) Associate Editor, Revista Chilena de Historia Natural (2007-2011) and Journal of Mammalogy (2011-present).

(2) I have coordinated three international symposia, most recently Social instability: Direct fitness consequences and underlying physiological mechanisms (2018). European Conference on Behavioral Biology (Liverpool, U.K.).

(3) Grant-writing training. Eighteen of my students have received 33 grants from university, state, and societal funding programs as well as from NSF EASPI and NSF DDIG.

(4) I have coordinated two Journal of Mammalogy Special Features, the most recent one was on long-term studies on mammals (2017, vol. 98, no. 3). Contributors included faculty and students from the Americas, Africa, and Europe.

(5) STEM Education activities include teaching undergraduate and graduate courses, coauthoring three science education papers with students, contributing to the design of a prairie dog exhibit at the Chattanooga Zoo (with UTC College of Engineering students), and training >30 U.S. research students in Chile.

NAME: Jin Wang

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)
University of Science & Technology of China	Hefei, Anhui	Mathematics	B.S.	1998
University of Science & Technology of China	Hefei, Anhui	Applied Mathematics	M.S.	2000
Ohio State University	Columbus, OH	Applied Mathematics	Ph.D.	2004

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

From - To	Position Title, Organization and Location
2014 – present	Professor and UNUM Chair of Excellence in Applied Mathematics, University of Tennessee at Chattanooga, TN
2012 – 2014	Associate Professor of Mathematics, Old Dominion University, Norfolk, VA
2007 – 2012	Assistant Professor of Mathematics, Old Dominion University, Norfolk, VA
2005 – 2007	Assistant Research Professor of Mathematics, Duke University, Durham, NC
2004 – 2005	Lecturer of Mathematics, The Ohio State University, Columbus, OH

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

1. J. Wang, X. Zhang, and Q. Zhuang, An immersed Crouzeix-Raviart finite element method for Navier-Stokes interface problems, International Journal of Numerical Analysis and Modeling, 19(4): 563-586, 2022.

2. F. Bao, L. Mu, and J. Wang, A fully computable posteriori error estimate for the Stokes equations on polytopal meshes, SIAM Journal on Numerical Analysis, 57(1): 458–477, 2019.

3. Z. Cheng, Y. Liu, M. Zhang, and J. Wang, IB-WENO method for incompressible flow with elastic boundaries, Journal of Computational and Applied Mathematics, 362: 498–509, 2019.

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

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

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

1. Z. Cheng and J. Wang, Modeling epidemic flow with fluid dynamics, Mathematical Biosciences and Engineering, 19(8): 8334-8360, 2022.

2. C. Yang and J. Wang, Transmission rates and environmental reservoirs for COVID-19: A modeling study, Journal of Biological Dynamics, 15(1): 86–108, 2021.

3. C. Ratchford and J. Wang, Modeling cholera dynamics at multiple scales: environmental evolution, between-host transmission, and within-host interaction, Mathematical Biosciences and Engineering, 16(2): 782–812, 2019.

4. D. He, X. Wang, D. Gao, and J. Wang, Modeling the 2016-2017 Yemen cholera outbreak with the impact of limited medical resources, Journal of Theoretical Biology, 451: 80–85, 2018.

5. A. Timalsina, J. Tian, and J. Wang, Mathematical and computational modeling of tumor virotherapy with mediated immunity, Bulletin of Mathematical Biology, 79: 1736–1758, 2017

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

1. Served as a reviewer for about 60 research journals (over 100 manuscripts).

2. Organized the Interdisciplinary Mathematics Summer Camp for High School Students at UTC in four consecutive years (2016 – 2019).

3. Served as a grant review panelist for several funding agencies (including NSF and NIH) and reviewed more than 80 grant applications.

4. Developed four new graduate courses, including one for Mathematical Biology.

5. Mentored more than 40 graduate and undergraduate students, including 15 students from underrepresented groups.

NAME: Mina Sartipi

POSITION TITLE & INSTITUTION: Guerry Professor and PhD Program Coordinator, Computer Science and

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

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
Sharif University of Technology	Tehran, Iran	Electrical Engineering	BS	2000
Georgia Institute of Technology	Atlanta, GA	Electrical and Computer Engineering	MS	2003
Georgia Institute of Technology	Atlanta, GA	Electrical and Computer Engineering	PhD	2006
Harvard Business School	Boston, MA	Young American Leaders Program	Other training	2019

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

From - To	Position Title, Organization and Location
2020 - present	Guerry Professor and PhD Program Coordinator, Computer Science and Engineering Dept., University of Tennessee at Chattanooga
2017 - present	Founding Director, Center for Urban Informatics and Progress, University of Tennessee at Chattanooga
2018 - present	Faculty Member, Bredesen Center for Interdisciplinary Research and Graduate Education, University of Tennessee at Knoxville
2015 - 2020	UC Foundation Professor and PhD Program Coordinator, University of Tennessee at Chattanooga
2011 - 2015	UC Foundation Associate Professor , University of Tennessee at Chattanooga
2006 - 2011	Assistant Professor, Computer Science and Engineering Dept., University of Tennessee at Chattanooga

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

T. V. Tran and M. Sartipi, "Neuroevolution for transportation applications". The 11th International Workshop on Urban Computing at ACM SIGKDD conference on knowledge discovery and data mining, August 2022.

T. V. Tran, T. -N. Doan and M. Sartipi, "TSLib: A Unified Traffic Signal Control Framework Using Deep Reinforcement Learning and Benchmarking," 2021 IEEE International Conference on Big Data (Big Data), 2021, pp. 1739-1747, doi: 10.1109/BigData52589.2021.9671993

K. Kotobi and M. Sartipi, "A Novel Congestion Avoidance Algorithm for Autonomous Vehicles Assessed by Queue Modeling", International Journal of Interdisciplinary Telecommunications and Networking, Volume 11, Issue 2, April-June 2019.

J. Roland, P. D. Way, C. Firat, T. -N. Doan, M. Sartipi, "Modeling and predicting vehicle accident occurrence in

Chattanooga, Tennessee," Elsevier Journal of Accident Analysis & Prevention, Volume 149, 2021, 105860, ISSN 0001-4575.

Peter D. Way, Jeremiah Roland, Osama Osman, Mina Sartipi, "Spatio-Temporal Accident Prediction: Effects of Negative Sampling on Understanding Network-Level Accident Occurrence," Journal of Transportation Research Record, 2021.

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

R. Sen, A. K. Bharati, S. Khaleghian, M. Ghosal, M. Wilbur, T. V. Tran, P. Pugliese, M. Sartipi, H. Neema, and A. Dubey, "E-Transit-Bench: Simulation Platform for Analyzing Electric Public Transit Bus Fleet Operations", ACM International Conference on Future Energy Systems, June 2022.

Seyedmehdi Khaleghian, Himanshu Neema, Mina Sartipi, and Abhishek Dubey, "Calibration of Microscopic and Mesoscopic Traffic Simulation Model of a Large Scale Network Based on the Real World Speed Data". 101st Transportation Research Board Annual Meeting, No. TRBAM-22-01032, , January 2022.

A. Alharin, T. -N. Doan and M. Sartipi, "Reinforcement Learning Interpretation Methods: A Survey," in IEEE Access, vol. 8, pp. 171058-171077, September 2020.

A. Harris, M. Sartipi, "Data Integration Platform for Smart and Connected Cities," Proc. of ACM Smart City Operations and Platforms Engineering, April 2019.

A. Harris, J. Stovall, and M. Sartipi, "MLK Smart Cooridor: An Urban Testbed for Smart City Applications", Poc. of IEEE Big Data Conference, December 2019.

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

IEEE Senior Member

Faculty Advisor - 2016-present, Girls in Computer Science (GiCS)

Member of the board of directors for startups and non-profits

2019 Chattanooga Influencer- Chosen by the Edge, Chattanooga's Business Magazine, as the 2019 Chattanooga Influencer for her role in Smart City research and collaboration with city, county, and industry partners

Recipient of $4.5M from USDOT in collaboration with the City of Chattanooga, EPB (Chattanooga's power and telecommunication company), and industry partners to study nexus of transportation, energy, and people.

Farah Kandah

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

a. Professional Preparation

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

b. Appointments

- **UC Foundation Associate Professor and Graduate Program Coordinator** **Aug. 2018 – Present**
  Department of Computer Science and Engineering, University of Tennessee at Chattanooga
- **UC Foundation Assistant Professor and Undergraduate coordinator** **Aug. 2014 – July 2018**
  Department of Computer Science and Engineering
  University of Tennessee at Chattanooga
- **Assistant Professor** **Aug. 2012 – 2014**
  Department of Computer Science and Engineering
  University of Tennessee at Chattanooga
- **Teaching Assistant** **2011 – 2012**
  Department of Computer Science
  North Dakota State University
- **Research Assistant** **2009 – 2011**
  Department of Computer Science
  North Dakota State University
- **Lecturer and Course Coordinator** **2005 – 2007**
  Department of Computer Science
  The Hashemite University

c.i. Products Most Closely related to the Proposed Project

1. Jacob Coleman and Farah Kandah, "Towards Blockchained Authentication and Trust Management for Connected Autonomous Vehicles in Smart Cities", IEEE Consumer Communications and Networking Conference (CCNC) (*under review*).
2. Farah Kandah and Steven Schmitt, "SAND: Smart and Adaptable Networking Design Using Virtual Slicing over Software-Defined Network", Internet of Things.
3. Jacob Coleman, Farah Kandah, Steven Schmitt and Mohammed Akour, "Community Trust Distribution in Vehicle Ad-hoc Networks", *New Trends in Information Technology (NTIT 2017)*.
4. Farah Kandah and Jesse Whitehead, "Towards Trusted and Energy Efficient Data Collection in Unattended Wireless Sensor Networks", Springer – Wireless Networks (*under review*).
5. Farah Kandah and Jesse Whitehead, "Trust-based Survivability Provisioning in Wireless Mesh Networks", *IJIPM: International Journal of Information Processing and Management*, Vol. 7, No. 2, pp. 36 ~ 47, 2016

c.ii. Other Significant Publications

1. Farah Kandah, Steven Schmitt and Jesse Whitehead, Using Hybrid Spectrum Handoff Towards Fairness Usage in Cognitive Radio Networks, *International Journal of Information Processing*

and Management (IJIPM 2017).
2. Jesse Whitehead, Farah Kandah: Cluster-Based Dynamic Backup in Cognitive Radio Networks, *the IEEE ICNC - Workshop on Computing, Networking and Communications (CNC). 2016*
3. Farah Kandah, and Jesse Whitehead: Energy-aware Multipath Provisioning in Wireless Mesh Networks, *Consumer Communications and Networking Conference (CCNC 2015)*.
4. Farah Kandah, Yashaswi Singh, Weiyi Zhang and Yulu Ma: Mitigating Misleading Routing Attack using Path Signature in Mobile Ad-Hoc Networks, *Global Communications Conference (GLOBECOM), 2013 IEEE*, pp.617-622, 2013.
5. Farah Kandah, Yashaswi Singh, and Weiyi Zhang: Mitigating Colluding Injected Attack using Monitoring Verification in Mobile Ad-hoc Networks, *Security and Communication Networks (SCN), Wiley*, 6, pp. 539-547, 2013. Farah Kandah, Yashaswi Singh, and Weiyi Zhang: Mitigating Eavesdropping Attack using Secure Key Management Scheme in Wireless Mesh Networks, *Journal of Communications*, 7, pp. 596-605, 2012.

d. Synergistic Activities

- Dr. Kandah is a member of the IEEE, IEEE Computer Society and IEEE Communication Society (ComSoc).
- Founder of the Network Communication Laboratory (NCL) at UTC (Aug 2012), which conducts research in the fields of Cyber physical, Cybersecurity systems, smart communications, and smart cities.
- Dr. Kandah is currently working with collaborators to establish an IoT Laboratory at UTC, which will focus on research in the fields of Cyberphysical and Cybersecurity systems.
- An active researcher in the community and is currently serving on a number of conferences and as a TPC member, reviewer, and chair.
- Dr. Kandah is the recipient of the Outstanding Teaching Award for two consecutive years and was named the Computer Science and Engineering Outstanding Researcher in 2016.

NAME: Osama A. Osman

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

A. PROFESSIONAL PREPARATION

INSTITUTION	LOCATION	MAJOR/AREA OF STUDY	DEGREE (if applicable)	YEAR (YYYY)
Cairo University	Egypt	Civil Engineering (Honors)	B.S.	2006
Cairo University	Egypt	Civil Engineering	M.S.	2010
Louisiana State University	Louisiana, USA	Civil Engineering	Ph.D.	2015

B. APPOINTMENTS

From - To	Position Title, Organization and Location
2019 ~	Assistant Professor - Civil and Chemical Engineering Department - University of Tennessee at Chattanooga - Chattanooga, TN, USA
2018 - 2019	Research Faculty - Virginia Tech Transportation Institute - Blacksburg, VA, USA
2016 - 2018	Research Associate - Louisiana State University - Baton Rouge, LA, USA
2016-2016	Adjunct Professor - Louisiana State University - Baton Rouge, LA, USA
2006 - 2010	Sr. Transportation Engineer - Cairo, Egypt

C. PRODUCTS

1. Karbalaieali, S., O. A. Osman, and S. Ishak. A Dynamic Cooperative Merging Control Algorithm for Connected Automated Vehicles. IEEE Transactions on Intelligent Transportation Systems, Vol. 21, no. 10, 2020, pp. 4111-4122.
2. Osman, O. A. and H. Rakha. Application of Deep Learning for Characterization of Drivers' Engagement in Secondary Tasks in In-Vehicle Systems. Transportation Research Record, Vol. 2674, no. 8, 2020, pp. 429-440.
3. Ahmed, S., O. A. Osman, and J. Codjoe. Mitigating Traffic Congestion on I-10 Mississippi River Bridge in Baton Rouge, LA. In MATEC Web of Conferences, vol. 271, p. 06002. EDP Sciences, 2019.
4. Wan, L., D. Cheng, R. Bian, S. Ishak and O. A. Osman, 2017. Accounting for Travel Time Reliability, Trip Purpose and Departure Time Choice in an Agent-Based Dynamic Toll Pricing Methodology. IET Intelligent Transport Systems, 12(1), pp.58-65.
5. Osman, O.A. and S. Ishak, 2016. Genetic Algorithm–Based Approach for Optimal Deployment of Roadside Units in Connected and Automated Vehicle Environments. Transportation Research Record, 2595(1), pp.139-147.

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

#1. Osman, O.A. and S. Ishak, 2015. A network level connectivity robustness measure for connected vehicle environments. Transp. Res. Part C: emerg. techno., 53, pp.48-58. #2. Osman, O.A., M. Hajij, P. R. Bakhit, and S. Ishak, 2019. Prediction of Near-Crashes from Observed Vehicle Kinematics using Machine Learning. Trans. Res. Record, p.0361198119862629. #3. Mousa, S.R., P. R. Bakhit, O. A. Osman, and S. Ishak, 2018. A Comparative Analysis of Tree-Based Ensemble Methods for Detecting Imminent Lane Change Maneuvers in Connected Vehicle Environments. Transp. Res. Record, 2672(42), pp.268-279. #4 Osman, O. A., J. Codjoe, S. Ishak, J. Rodriguez, and M. Russell, 2015. Long-term evaluation of the operational performance of fixed time ramp metering control strategy: a freeway corridor study. Canadian Journal of Civil Engineering, 42(11), pp.910-918.

D. SYNERGISTIC ACTIVITIES

• Chair, Communication Subcommittee of the Transportation Research Board (TRB) Standing Committee on Artificial Intelligence and Advanced Computing Applications in Transportation (2018 – present)
• Member of the Society of Automotive Engineers' Committee on Cooperative Driving Automation
• Active Reviewer for major international transportation journals including Transportation Research Part C, IEEE Transactions of ITS, Big Data, and Intelligent Vehicles, Accident Analysis and Prevention, Safety Research, and Intelligent Transportation Systems
• Troy H. Middleton Scholarship Award
• Best Paper Award on User Information Systems at the 2020 Annual Meeting of the Transportation Research Board, Washington D.C.

Dr. Stephanie L. DeVries
Assistant Professor of Hydrology and Aquatic Geochemistry
Department of Biology, Geology, and Environmental Science, MP 2653
University of Tennessee at Chattanooga, Chattanooga, TN 37403
Phone: (423) 425-4341
Email: stephanieldevries@gmail.com

a. Professional Preparation

Grinnell College	Grinnell, IA	Art	BA, 1999
City College of New York	New York, NY	Geology	MA, 2010
CUNY Graduate Center	New York, NY	Earth/Env. Sci	PhD, 2017
University of Wisconsin	Madison, WI	Hydrogeology	Post-doc, 2019

b. Appointments

2019- Asst. Professor of Hydrology and Aquatic Geochemistry, University of Tennessee at Chattanooga
2018-2019 Water Science and Policy Fellow (Hydrogeology), University of Wisconsin at Madison
2017-2018 Adjunct Assistant Professor, City College of New York at NY, NY
2012-2018 College Lab Technician, City College of New York at NY, NY
2012-2016 Physical Scientist Intern, US Geological Survey at Woods Hold, MA
2008-2017 Adjunct Lecturer, City College of New York at NY, NY

c. Publications

DeVries, S., Zhang, P. (2016). Antibiotics and the Terrestrial Nitrogen Cycle: A Review. Current Pollution Reports, 2, 51-67.

DeVries, S. L., Loving, M., Li, X., & Zhang, P. (2015). The effect of ultralow-dose antibiotics exposure on soil nitrate and N_2O flux. Scientific Reports, 5, 16818.

Chen, C., Li, J., DeVries, S. L., Zhang, P., & Li, X. (2015). Transport of antibiotic resistance plasmids in porous media. Vadose Zone Journal, 14(3).

DeVries, S.L. W. Liu, N. Wan, P. Zhang & Li, X. (2012). Biodegradation of MIB, geosmin, and microcystin-LR in sand columns. Water Science and Technology, 12(5), 691-698.

Zhang, P., DeVries, S. L., Dathe, A., & Bagtzoglou, A. C. (2009). Enhanced mixing and plume containment in porous media under time-dependent oscillatory flow. Environmental science & technology, 43(16), 6283-6288.

d. Synergistic Activities

Member, State of Wisconsin's Legislative Task Force on Nitrogen Pollution, 2019

e. Collaborators & Other Affiliations

(i)Collaborators

D. Hart, Department of Extension (WGNHS), University of Wisconsin-Madison.

K. Bradbury, Department of Extension (WGNHS), University of Wisconsin-Madison.

K. McDonald, Department of Earth & Atmospheric Sciences, City College of New York

M. Cardiff, Department of Geology, University of Wisconsin-Madison

P. Juckem. United States Geological Survey, Madison, WI.

P. Zhang, Department of Earth & Atmospheric Sciences, City College of New York

S. Mauel, Department of Extension (WGNHS), University of Wisconsin-Madison.

(ii) Graduate and Postdoctoral Advisors

P. Zhang, graduate advisor, Dept of Earth & Atmospheric Sciences, City College of New York.

K. Bradbury, postdoctoral sponsor, Dept of Extension (WGNHS), University of Wisconsin-Madison.

M. Cardiff, postdoctoral sponsor, Dept of Geology, University of Wisconsin-Madison.

f. Research Impacts

Modeling research in Wisconsin (technical report pending) has led to a review of state policy related to easements around well-head protection areas.

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.

Wang-Yong Yang
Assistant Professor
615 McCallie Ave, Chattanooga, TN 37403
423-425-5771
wangyong-yang@utc.edu

(a) Professional Preparation

Pusan National University	Busan, Korea	Chemistry	B.S. 1996
Pusan National University	Busan, Korea	Chemistry	M.S. 1998
Florida State University	Tallahassee, FL	Chemistry	Ph.D. 2011
Scripps Research Institute	Jupiter, FL	Chemical Biology	Postdoc 2011-2016

(b) Appointments

Assistant Professor, University of Tennessee Chattanooga 2018-present
Research Scientist, Dong-Wha Pharm. Co. Ltd., Korea 1998-2003

(c) Products Products Most Closely Related to the Proposed Project

Yang, W.-Y.; He, F.; Strack, R. L.; Oh, S. Y.; Frazer, M.; Jaffrey, S. R.; Todd, P. K.; Disney, M. D. **Small Molecule Recognition and Tools to Study Modulation of r(CGG)^{exp} in Fragile X-Associated Tremor Ataxia Syndrome.** *ACS Chem. Biol.* **2016**, *11*, 2456.

Yang, W.-Y.; Gao, R.; Mark, S.; Sarkar, P.; Disney, M. D. **Studying Small Molecule Recognition of RNA Base Pairs Enables the Design of a Bioactive Small Molecule that Targets r(AUUCU) Repeats in Spinocerebellar Ataxia 10.** *Nat. Commun.* **2016**, *7*, 11647.

Yang, W.-Y.; Wilson, H. D.; Velagapudi, S. P.; Disney, M. D. **Inhibition of Non-ATG Translational Events in Cells via Covalent Small Molecules Targeting RNA.** *J. Am. Chem. Soc.* **2015***, 137,* 5336

Su, Z.; Zhang, Y.; Gendron, T. F.; Bauer, P. O.; Chew. J.; Yang, W.-Y.;, Fostvedt, E.; Jansen-West, K.; Belzil, V. V.; Desaro, P.; Johnston, A.; Overstreel, K.; Oh, S.-Y.; Todd, P. K.; Berry, J. D; Boeve, B. F.; Dickson, D.; Floeter, M. K.; Traynor, B. J.; Morelli, C.; Ratti, A.; Silani, V.; Rademkers, R.; Brown, R. H.; Rothstein, J. D.; Boylan, K. B.; Petrucelli, L.; Disney, M. D. **Biomarker and lead small molecule discovery to target r(GGGGCC)-associated defects in c9FTD/ALS.** *Neuron* **2014**, 83, 1043

Colak, D.; Zaninovic, N.; Cohen, M. S.; Rosenwaks, Z.; Yang, W.-Y.; Gerhardt, J.; Disney, M. D.; Jaffrey, S. R. **Promoter-bound trinucleotide repeat mRNA drives epigenetic silencing in Fragile X syndrome.** *Science* **2014**, *343*, 1002.

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

Disney, M. D.; Liu, B.; Yang, W.-Y.; Tran, T.; Sellier, C.; Childs-Disney, J. L.; Charlet-Berguerand, N. **A Small Molecule that Targets r(CGG)^{exp} and Improves Defects in Fragile X-Associated Tremor Ataxia Syndrome.** *ACS. Chem. Biol*. **2012**, *7*, 1711.

Yang, W.-Y.; Breiner, B.; Kovalenko, S. V.; Ben, C.; Singh, M.; LeGrand, S. N.; Sang, A. Q.-X.; Strouse, G. F., Copland, J. A.; Alabugin I. V. **C-Lysine Conjugates: pH-Controlled Light-Activated Reagents for Efficient Double Stranded DNA Cleavage with Implications for Cancer Therapy.** *J. Am. Chem. Soc.* **2009**, *113*, 11458.

Yang, W.-Y.; Marrone, S. A.; Minors, N.; Zorio, D. A. R.; Alabugin, I. V. **Fine-tuning alkyne cycloadditions: Insights into photochemistry responsible for the double-strand DNA-cleavage via structural perturbations in diaryl alkyne conjugates.** (*Beilstein J. Org. Chem.* **2011**, *7*, 813.)- invited article, special issue on photocycloadditions.

Yang, W.-Y.; Roy S.; Phrathep, B.; Rengert, Z.; Kenworthy, R.; Zorio, D. A. R.; Alabugin, I. V. **Engineering pH-Gated Transitions for Selective and Efficient Double Strand DNA Phtocleavage in Hypoxic Tumors.** *J. Med. Chem.* **2011**, *54*, 8501.

Haify, S.N.; Buijsen, R.A.M.; Verwegen, L.; Severijnen, E.A.W.F.M.; de Boer, H.; Boumeester, V.; Monshouwer, R.; Yang, W.Y.; Cameron, M.D.; Willemsen, R.; Disney, M.D.; Hukema, R.K. **Small molecule 1a reduces toxic FMRpolyG levels in in vitro and in vivo models for FMR1 premutation.** *Hum. Mol. Genet*. **2020**. *30*, 1632.

(d) Synergistic Activities

1. Summer undergraduate research program organizer (2018-Present). Prior to the summer, Dr. Yang organizes the application process, and at the end of the summer organizes a departmental poster session (open to the campus) in preparation for the students to present their work at a conferences. During the summer, Dr. Yang organizes the meetings, student presentations, inviting a summer speaker, tours of local chemical industry and workshops on campus such as Endnote tutorials done through the library.

2. Interdisciplinary projects. Research interest has focused on bioactive organic molecules, specifically the development of target-selective organic compounds controlled by an external stimulus such as light and pH. Bio-related multidisciplinary research is one of the most attractive topics for undergraduate students majoring in natural science fields and this research field will surely meet their intellectual demands

3. Mentored over 25 undergraduate research students (2007-Present). Notable undergraduate achievements are as follows.

- Fisher Fellowship from the American Cancer Society (2007)
- NSF Graduate Fellowship (2013)
- 1st place poster award (87th Florida ACS Annual Meeting and Exposition, 2011)
- Three publications with six undergraduate students

ABDOLLAH (ABI) ARABSHAHI
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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.”

Appendix B

Awardee Project Reports
FY 2022

Fiscal Year 2022 Final Project Report

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

Yunye Shi, Lead PI

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

Project Title: “Predicting biomass gasification output: A machine learning approach”

Date Submitted: 09/02/2022

Award Start—End Date: September 1, 2020–June 30, 2022

Non-Technical Summary:

Gasification is an effective thermochemical conversion process. It transforms solid biomass into combustible gases, i.e., mixture of hydrogen, methane, carbon monoxide, carbon dioxide, light hydrocarbons, and char. The produced gaseous mixture, known as syngas, can be used directly combusted to generate electricity and power or further converted into various biofuels. The flexibility of syngas endues makes gasification a very promising technology. Accurate prediction of biomass gasification outcome is a critical step to achieve efficient system design and optimal operations. For this purpose, various kinetics and equilibrium models have been developed. However, the assumptions made in these models significantly limit the practical usability and consistency. The proposed research develops models via machine learning approaches to predict gasification output. The predicted results are compared with experimental data for model validation. The work is through collaboration with the Federal University of Itajuba NEST Lab in Brazil.

PROJECT TITLE: Predicting biomass gasification output: A machine learning approach
Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH

Various regression machine learning models are developed including linear models, artificial neural networks (ANNs), support vector machine (SVM), and tree-based models. K-folds validation approach are applied for parameter tuning. Models are validated against experimental data and are cross-compared.
List of tasks:

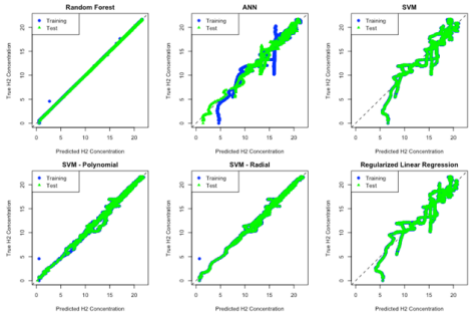
- Experimental data collection
- Machine learning model development, model training, and testing
- Gasification output prediction and operational optimization

OUTCOMES

- The project has developed machine learning models that could be used for not only gasification, but other nonlinear processes for future study
- Paper titled "Predicting Steam-Gasification Output Using Artificial Neural Networks" has been accepted for IMECE 2021 for both publication and conference presentations
- Paper titled "Predicting Steam-Gasification Output via Machine Learning Approaches" is under review in the International Journal of Hydrogen Energy.

RESULTS

All models had good performance except for regularized linear regression and support vector regression with linear kernels. This is consistent with the highly heterogeneous and non-linear nature of the gasification process. Although SVR is different from linear regression by minimizing generalization error bound rather than the sum of squared errors between prediction and actual outputs, SVR with linear kernel maps feature vector into hyperplane with linear separation. The RF method, rooted from decision tree models, has no pre-determined functions. RF methods construct multiple decision trees at the training time and outputting the mean prediction of the individual trees to reduce high variance generated from each tree.



OTHER INFO

Budget and Schedule

Total Budget:	$15,000.00
Actual Used (Year 1):	$ 13,101.33
Balance:	$1,898.67

Approved carryover for 2021 and 2022 fiscal years (Due to COVID-19): $1,898.67

Total period of performance is 24 months.
Task 1: Months 1-4: Data collection and preprocessing
Task 2: Months 4-12: Model building and testing
Task 3*: Months 12-24: Report generation and publications
*Extended due to COVID-19

Deliverables

- Weekly meeting with students and monthly progress report
- Final report detailing results, financials, and future work.
- Publications and external and internal conference presentations.

Organization Information

Dept 2452, 615 McCallie Ave | Chattanooga, TN 37403, Ph: 423-425-2256
Email: Yunye-shi@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Data collection and data preprocessing	A data base with 16,000 data points was constructed to train models and to test model accuracy.
Random forest model	Six machine learning models were utilized to predict the output of biomass gasification including syngas composition and lower heating value of the syngas. All models had good performance except for linear regression, regularized linear regression and support vector regression with linear kernels. This is consistent with the highly heterogeneous and non-linear nature of the gasification process. The RF model outperformed the others for all output variable predictions. As a model rooted from decision tree models, RF method has no pre-determined functions, each decision is made based on an "if-else" logic. In random forests, the number of features that can be split on each node is limited by the hyper-parameter so that the model does not rely too heavily on any individual feature, and it makes fair use of all potential predictive features. In addition, each tree draws a random sample from the original data set during training splitting, which adds a further element of randomness that prevents overfitting. Because of the above reasons, RF regression shows great performance in predicting gasification outputs and it is an effective method for estimating missing data.
ANN model	
SVM model	
SVM model with polynomial kernel	
SVM model with radial kernel	
Regularized regression model	

Challenges & Strategies Used to Address / Overcome:

Since machine learning models need large datasets to train models, challenges of the data collection are time and cost consuming. The data used in the project is collected at the University of Itajuba in Brazil. But due to COVID-19 travel restrictions, data collection could only be done by the partner's team, which is how the first task was accomplished.

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

The proposed conventional models show great results. Therefore, there has been a little shift of the work from developing RNN models to applying the six regression models to more areas.

IMPACT & OUTCOMES

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

Prior to joining UTC, I have been constantly working with the team from the Federal University of Itajuba NEST Lab in Brazil. The NEST group in Brazil is well known for their excellent work in cogeneration and distributed generation from renewable energy sources (biomass and solar). More than three papers have been generated from the collaboration on studying biomass gasification. The proposed project further promoted the collaboration and enhanced interpersonal communication. This project has sparked many more new ideas between the teams.

Students Impacted

Brenan Ward: The student worked on the project for over 3 months and developed a basic understanding of machine learning. Brennan is seeking further opportunities to stay in the team for graduate study.

Hannah Morgan: The student was introduced to the project during her junior year and did data analysis for the project.

Greg Johnson: The student worked on the project during his senior year (Fall 2021—Spring 2022). He has converted the code developed in R into Python. During the process, the student successfully used the coding skills he learned from class into a new topic. He presented the work at both UTC Tech Symposium and NCUR.

Community and Broader Impacts

Biomass utilization is a promising technology to partly replace fossil fuel combustion in power plants. It is environmentally friendly in many different aspects: CO2 neutral, less NOX production, and so on. Accurately predicting syngas output not only benefits system design and operation, but it also helps with reducing time and cost in the process. Machine learning based methods, because of the unique feature that is not design based, has the potential to be widely used in output prediction in energy conversion processes.

Scholarly Products

External Conferences:

1. Shi, Y., Maya, D., Ratner, A. Predicting Steam-Gasification Output Using Artificial Neural Networks. ASME International Mechanical Engineering Congress and Exposition 2021.
2. Johnson, G., Shi, Y. Prediction of Gasification Outputs via Machine Learning Approaches. National Conference on Undergraduate Research NCUR 2022.
3. Ward, B., Shi, Y. Prediction of Gasification Outputs via Supervised Learning Approaches. National Conference on Undergraduate Research NCUR 2021.

Presentations at UTC:

- Johnson, G., Shi, Y. Prediction of Gasification Outputs via Machine Learning Approaches. UTC College of Engineering Tech Symposium 2022.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

A new project has been initiated with Professor Diego Yepes Maya from the Federal University of Itajuba in Brazil. The project is to apply the developed models from the current project to a different research question.

EXTERNAL FUNDING

Proposal Submissions

- Impact of Additives on Combustion of Bio-derived Fuels. Agency: NSF ERI. Duration: 09/2023–07/2025. Total amount: $199,523. Role: Principal Investigator. Submission in preparation.
- Impact of Additives on Combustion of Bio-derived Fuels. Agency: NSF ERI. Duration: 09/2022–07/2024. Total amount: $199,523. Role: Principal Investigator. Not funded.
- Impact of Additives on Combustion of Bio-derived Fuels. Agency: DOE ORAU Ralph E. Powe Junior Faculty Enhancement Awards. Total amount: $5,000. Role: Principal Investigator. Not funded.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

- NSF grant webinars
- College grant writing workshops

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 follow up my CEACSE grant with the following work within next three years:

- Publish 1-2 journal articles based on the obtained results.
- Extend the work into new areas: combine the developed machine learning models with CFD models to improve the accuracy of gasification output predictions and apply the developed models to biomass torrefaction.
- Submit external proposals to NSF and DOE.

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

I will continue to work with my current collaborator from the Federal University of Itajuba NEST Lab in Brazil. At the same time, we will work on extending the area to include more faculty in the institutions to form a more divergent team.

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

The barriers that I foresee are the availability of external research funds and the balance between research and other duties.

FINANCIAL ACCOUNTING

All funds have been spent.

Fiscal Year 2022 Final Project Report

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

Dr. A.K.M. Azad Hossain, Lead PI

Co-PI(s): Dr. Jejal Reddy Bathi and Dr. Mark Schorr
Other Personnel: Richard Blanton, Graduate Research Assistant, Caleb Mathias - Undergraduate Research Assistant, Connor Firat - Graduate Research Assistant, Shuvashish Roy - Graduate Research Assistant, and Syed Tareq - Graduate Research Assistant.

Project Title: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"

Date Submitted: 09/02/2022

Award Start—End Date: July 1, 2019–June 30, 2022

Non-Technical Summary:

Satellite observations have been used for water quality studies for many years, but they provide only surface observations and challenges related to cloud coverage, ground truthing, and variable spatial and temporal resolutions remain. Numerical models can provide hydrodynamically computed water quality data on the water surface as well as in the water column, but they have issues with initializations, boundary conditions, calibration, and validation. Although both methods have weaknesses when used together, they can become a powerful tool to study surface water quality. The proof of concept of this capability was demonstrated in Enid Lake, MS; Lake Pontchartrain, LA; and the Mississippi River in the National Center for Computational Hydroscience and Engineering at the University of Mississippi. The primary objective of this project was to further explore this capability at the University of Tennessee at Chattanooga by using the EPA's hydrodynamic and watershed models coupled with NASA's Earth Observations Satellite imagery and near real time field measurement to study the spatio-temporal variability of hydrodynamically computed surface water quality parameters in the watersheds of southeast Tennessee.

The accomplishments of this project include: (1) collection of in situ water quality measurements in selected parts of the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek; (2) collection of different multispectral satellite imagery; (3) development of different satellite observed water quality estimation models for the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek; (4) estimation of remote sensing based water quality parameters including turbidity, chlorophyll, conductivity, pH, and dissolved oxygen; (5) generation of a complete bathymetric digital elevation model for the Tennessee River; (6) development of EFDC 3D model for the Tennessee River flows (flow depth, flow velocity, and flow quantity); and (7) delineation and initial set-up of watershed hydrology and pollution simulation model, using the EPA's BASINS Program. In addition to these accomplishments, this project enhances the capability of the Geological and Environmental Remote Sensing Laboratory (GERSLab) at UTC by providing new water quality measuring equipment and resources.

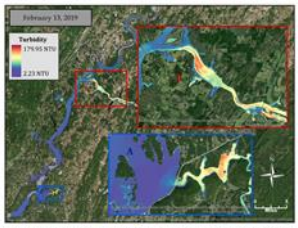
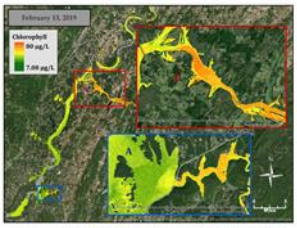
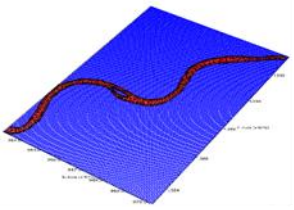
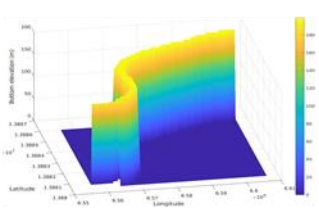
This project produced several conference presentations, a book chapter, provided research data and results for preparing several journal articles, and seeking external funding opportunities. Three graduate students and one undergraduate student worked on this project. All of the students have graduated and already accepted different professional positions and started pursuing further higher education.

The city of Chattanooga, TN has grown substantially during the last several decades and has become the center of a series of urbanized sub-watersheds. The environmental impacts, especially the quality of surface waters due to this growth, have become a major concern for the sustainable developments of the Greater Chattanooga area. This project, provided with the potential proof of concept of satellite-based remote sensing-integrated water quality modeling capability, would provide a powerful tool to study the impacts of land use and land cover change on the surface water quality in the watersheds of southeast Tennessee. The obtained results of this project would also provide a unique approach to study surface water quality in other areas in the United States and the rest of the world as well.

This project supports and contributes significantly to advance the SimCenter's mission in the environment research thrust by developing new innovative research at UTC on surface water quality modeling and simulation.

PROJECT TITLE: Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies

Technology Area of Interest: Environmental Sustainability and Climate Systems

TECHNICAL APPROACH	OUTCOMES
Integration of satellite observations with numerical models to estimate hydrodynamically computed surface water quality parameters in the watersheds of southeast Tennessee. List of tasks: (1) Geospatial/satellite data acquisition and processing (2) In situ water quality data acquisition (3) Remote sensing-based water quality estimation (4) Numerical model development and application (5) Water quality parameters estimation using numerical model coupled with satellite observations (6) Report generation and publications	The outcomes of this project include (1) one externally funded project, three additional external proposal submissions, one journal article, one book chapter, one conference proceeding article, 8 external conference presentations, and 3 internal (UTC) research presentations. Three manuscripts are in preparation for peer reviewed publications, along with research data and results for preparing several journal articles, and seeking external funding opportunities; (2) potential proof of concept of remote sensing integrated water quality modeling capability; and (3) support and contribution to advance the SimCenter's mission in the Environmental Sustainability and Climate Systems research thrust by developing new innovative research at UTC on surface water quality modeling and simulation.
RESULTS	**OTHER INFO**
Developed satellite observed water quality estimation models for the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek.  Estimation of Turbidity using Landsat 8 OLI image acquired on February 13, 2019  Estimation of Chlorophyll concentration using Landsat 8 OLI image acquired on February 13, 2019 Developed EFDC 3D model for the Tennessee River flows (flow depth, flow velocity, and flow quantity). EFDC Model Grid  Bathymetry of the Tennessee River 	**Budget and Schedule** Total Budget: $96,488.00 Actual Used (Year 1): $78,620.94 Balance: $17,867.06 Approved carryover for 2021 and 2022 fiscal years (Due to COVID-19): $14,200.00 Total period of performance is 36 months. Task 1: Months 1-8, Task 2: Months 1-8 Task 3: Months 1-9, Task 4: Months 1-8 Task 5*: Months 8-11 (+24 months), Task 6*: Months 3-12 (+24 months) * Extended due to COVID-19. **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work. • Publications and external and internal conference presentations. **Organization Information** Dept. 2653, 615 McCallie Avenue, Chattanooga, TN 37403, Ph: 423-425-4404 Email: azad-hossain@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

The city of Chattanooga, TN has grown substantially during the last several decades and has become the center of a series of urbanized sub-watersheds. The environmental impacts, especially the quality of surface waters due to this growth, have become a major concern for the sustainable developments of the Greater Chattanooga area. The water quality modeling capability of this project provides a powerful tool to study the impacts of land use and cover change on the surface water quality in the watersheds of southeast Tennessee. Data gathered through this study augment the scientific understanding of stream ecology in urban landscapes and, on a local scale, evaluates long-term effects of watershed/riparian land use practices and site-specific stream mitigation projects implemented by multiple agencies in an effort to maintain healthy streams in the Chattanooga area.

The accomplishments of this project include: (1) collection of in situ water quality measurements in selected parts of the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek; (2) collection of different multispectral satellite imagery; (3) development of different satellite observed water quality estimation models for the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek; (4) estimation of remote sensing based water quality parameters including turbidity, chlorophyll, conductivity, pH, and dissolved oxygen; (5) generation of a complete bathymetric digital elevation model for the Tennessee River; (6) development of EFDC 3D model for the Tennessee River flows (flow depth, flow velocity, and flow quantity); and (7) delineation and initial setup watershed hydrology and pollution simulation model, using the EPA's BASINS Program. Along with these accomplishments, this project enhanced the capability of GERSLab by providing new water quality measuring equipment and resources. This research advances BGE, College of Art and Sciences, School of Engineering, and University Strategic Plan goals to involve students in meaningful experiential learning and to be an engaged metropolitan university conducting innovative research of local, regional, and national interests.

<table>
<tr><th>List of Objectives / Aims / Major Milestones Proposed</th><th>Cumulative Outcomes / Accomplishments</th></tr>
<tr><td>Task 1.
Geospatial/satellite data acquisition and processing</td><td>Collection and processing of different multispectral satellite imagery. The acquired and processed satellite imagery are as follows:
One scene of Landsat 8 OLI multispectral image acquired over part of the Tennessee River on August 15, 2019.
Several scenes of high-resolution multispectral images acquired by the Plant Dove satellites (PlanetScope) over part of the Tennessee River on August 14–16, 2019 and October 22, 2019.
One scene of Sentinel-2 multispectral imagery acquired over the Tennessee River on October 22, 2019.</td></tr>
<tr><td>Task 2. In situ water quality data acquisition</td><td>Collection of in situ water quality measurements in selected parts of the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek.
Acquired near real-time (with satellite image acquisition) in situ water quality data (temperature, pH, turbidity, chlorophyll, dissolved oxygen, and conductivity) for about 30 stations in and around South Chickamauga Creek on August 15, 2019 and for about 50 stations in the Tennessee River near downtown and around South Chickamauga Creek on October 22, 2019.</td></tr>
<tr><td>Task 3. Remote sensing-based water quality estimation</td><td>Development of different satellite observed water quality estimation models for the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek.
A series of numerical models have been developed to estimate turbidity, chlorophyll, conductivity, pH, and dissolved oxygen (DO) using Landsat 8 OLI imagery (Task 2) and concurrent in situ water quality measurements (Task 1). The following table shows the selected regression equations and correlation coefficients for each water quality parameter.
<table>
<tr><th>Parameter</th><th>Band(s)</th><th>Regression Type</th><th>Equation</th><th>R^2</th></tr>
<tr><td>Turbidity</td><td>4</td><td>Nonlinear Exponential</td><td>$Turbidity = 1.769 * e^{0.284 * \rho_{red}}$</td><td>0.95</td></tr>
<tr><td>Chlorophyll</td><td>1,2,3</td><td>Linear Multi-Regression</td><td>$Chlorophyll = 10.37 + 29.55 * \rho_{coastal} - 39.41 * \rho_{blue} + 12.90 * \rho_{green}$</td><td>0.66</td></tr>
<tr><td>DO</td><td>5</td><td>Nonlinear Power</td><td>$DO = 11.405 * \rho_{NIR}^{-0.11}$</td><td>0.72</td></tr>
<tr><td>Conductivity</td><td>5</td><td>Nonlinear Exponential</td><td>$Conductivity = 181.64 * e^{-0.069 * \rho_{NIR}}$</td><td>0.45</td></tr>
<tr><td>pH</td><td>2,3,4</td><td>Linear Multi-Regression</td><td>$pH = 7.716 - 0.165 * \rho_{blue} + 0.145 * \rho_{green} - 0.076 * \rho_{red}$</td><td>0.42</td></tr>
</table>
Several numerical models have also been developed to estimate selected water quality parameters using Sentinel-2 and Planetscope imagery (Task 2) and concurrent in situ water quality measurements (Task 1).</td></tr>
</table>

Task 4. Numerical model development and application	As a part of this task, a detailed hydrological watershed model using the Hydrological Simulation Program—FORTRAN (HSPF) model for the South Chickamauga Creek watershed was developed such that the watershed hydrology and water quality can be simulated on a continuous basis. However, in order to simulate lateral discharges into the Tennessee River, with synchronized efforts with another CEACSE project, a detailed HSPF watershed model was also set up for North Chickamauga Creek. Both of these watersheds are located below the Chickamauga Reservoir. As part of this task, in collaboration with research funded by the United States Geological Survey through the Tennessee Water Resources Research Institute, a three-dimensional hydrodynamic model was developed and calibrated for a portion of the Tennessee River such that fate and transport of water quality parameters in the river can be quantified. The model developed using Environmental Fluid Dynamic Code (EFDC) was calibrated for hydraulics by comparing monitored flows and flow depth in the river. However, the model is yet be calibrated for water quality parameters.
Task 5. Water quality parameters estimation using numerical model coupled with satellite observations	Due to COVID-19 pandemic, this task remained partially incomplete. The obtained no-cost extension and approved carry-over fund used to make significant progress for this task including a complete laboratory setup for estimating total suspended sediments (TSS) estimation and field sample collection resources.
Task 6. Report generation and publications	Three quarterly progress reports and one annual report were prepared and submitted to report the progress of the project. The project produced one journal article, one book chapter, one conference proceeding article, 8 external conference presentations, and 3 internal (UTC) research presentations. Three manuscripts are in preparation for peer reviewed publications. Several other manuscripts will also be prepared for peer reviewed publications.

Challenges & Strategies Used to Address / Overcome:

Challenges	Strategies Used to Address / Overcome
1. Sometimes it was very difficult to obtain a cloud free satellite imagery. It becomes even more challenging due to large temporal frequency of Landsat satellite missions (16 days).	Used other optical satellites of similar spectral characteristics (such as PlanetScope and Sentinel-2) in addition to the Landsat 8 satellite.
2. Frequent cloud coverage over the study site kept it challenging to acquire more in situ water quality measurements along with near real-time satellite imagery, especially after storm events.	Used other optical satellites of similar spectral characteristics (such as PlanetScope and Sentinel-2) in addition to the Landsat 8 satellite.

3. The purchase of the new water quality measuring sonde was delayed as the paper works for procurement process took more time since the vendor was not registered with UTC.	Necessary efforts had been made to expedite the procurement process of the sonde. The sonde was finally received in early March 2020.
4. The watershed and hydrodynamic modeling have been delayed by the Co-PI's team.	Necessary efforts had been made to expedite the modeling efforts.
5. We had to postpone several field trips (to measure Nitrate, Chloride, and Ammonium) and laboratory work due to the current COVID-19 pandemic. These activities need to be resumed after summer to accomplish several proposed tasks of the project. These tasks are heavily dependent on the assistance of students/research assistants.	We requested to obtain a no-cost extension of the project and carry over some funds to support students' work and travels in the next fiscal year. We have received the approval of our request. Although it was really difficult to go to the field due to the continuation of the pandemic, we were able to collect some water samples for total suspended sediments (TSS) analysis.
6. The PI was supposed to attend the 2020 GSA Joint Section Meeting in Reston, VA in March to present some preliminary results of the project, but it was canceled due to the COVID-19 pandemic.	We attended the virtual GSA Section Meeting 2021 held in Auburn, AL on April 1–2, 2021.
7. The PI and students were supposed to attend the UTC Research Dialogue 2020 in April to present some preliminary results of the project, but it was canceled due to COVID-19 pandemic.	We submitted one poster on UTC's virtual scholar's platform and planned to present during future Research Dialogue events.

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

Satellite based water quality estimation models were developed to estimate turbidity on the basis of turbidity data collected in the field using water quality measuring sonde (Hydrolab HL7). However, the hydrodynamic models developed needed the input as suspended sediment concentration (SSC) instead of turbidity. This created a situation to convert the turbidity estimation to SSC for the EFDC model input. Arrangements had been made to measure SSC simultaneously with the in situ measurements of turbidity using Hydrolab HL7. We were supposed to have the measurements in the summer but due to the COVID-19 pandemic it was not possible. With the approval of the no-cost extension and carrying over some funds, we are planning to resume the field trips in fall 2020 and spring 2021.

IMPACT & OUTCOMES

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

Impact on the Career of the PI:

Research in water quality remote sensing is one of the major tasks of my laboratory, the Geological and Environmental Remote Sensing Laboratory (GERSLab) at UTC. The project provided funding to partly support a graduate student (graduate research assistant) and an undergraduate student (research assistant) for this research. These students' assistance was very critical to accomplish the completed tasks of this research. The partial summer salary in summer 2019 and summer 2020 provided me with the time that was necessary to process the research data and generate publishable results and thereby increased my capacity to successfully compete for tenure.

Candidates for tenure and promotion in the Department of Biology, Geology, and Environmental Science (BGE) must "establish an independent and externally recognized research program that involves students at UTC". This research facilitated achievement of this requirement because it involved UTC students, enabled data collection and analysis, and resulted in professional presentations and publications.

Along with these accomplishments, this project enhanced the capability of GERSLab by providing new water quality measuring equipment and resources.

Impact on the Career of the Co-PIs:

Dr. Mark Schorr was the PI of UTC's "Urban Streams Project" (1998–2000). This project provided him with the opportunity to explore the geospatial and hydrodynamic modeling efforts in similar research. He is the PI of the project that we recently started with TWRA as a continuation of "Urban Streams Project" (1998–2000).

Development of hydrodynamic and watershed modeling is a major focus of Dr. Jejal Bathi's laboratory. This project provided him with the funding to partly support two graduate students for this research. These students' assistance was instrumental to accomplish the completed tasks of this research. The partial summer salary in summer 2019 and 2020 provided him with the time that was necessary to process the research data and generate publishable results and thereby increased his capacity to advance his career in this area.

Students Impacted

Richard Blanton: Mr. Blanton is a graduate (MS) student in the Environmental Science program. He graduated in December 2019. He is currently working as a term research assistant for this project. He has been involved in water quality remote sensing research in the Geological and Environmental Remote Sensing (GERS) Laboratory at UTC for more than a year. This project provides him with the opportunity to continue participating in this research and experience how it can be integrated with numerical hydrodynamic and watershed models. This unique research experience helps him to become ready for pursuing further higher education and/or starting professional or research careers in this area. Recently Mr. Blanton has assumed

a GIS Analyst position at the Tennessee Valley Authority (TVA). Before joining the TVA, he worked at the GIS Department of Hamilton County, TN.

Caleb Mathias: Mr. Mathias is a recently graduated undergraduate student in Geology. He joined GERS Laboratory at UTC at the beginning of fall 2019 as a term research assistant for this project. This project provides him with the opportunity to conduct water quality remote sensing research and how it can be integrated with numerical hydrodynamic and watershed models. He is gaining valuable post baccalaureate research experience through this project. This unique research experience helps him prepare for pursuing higher education and/or starting professional or research careers in this area. Mr. Mathias has been admitted in the graduate program at the University of British Columbia (UBC) in Canada with full research assistantship. He will join UBC in fall 2021.

Connor Firat: Mr. Connor Firat is a graduate (MS) student in the Environmental Science program. He is currently working on his thesis research that integrates remote sensing technology with hydrodynamic models to estimate water quality parameters in the Tennessee River and adjacent creeks. He has been involved in water quality remote sensing research in the Geological and Environmental Remote Sensing (GERS) Laboratory at UTC for more than a year.

Abbie Faxon: Ms. Abbie Faxon is a recently graduated undergraduate student in Geology. Abbie graduated in Spring 2022 with a major in Geology and minor in Geographic Information Systems (GIS). Abbie successfully defended her Departmental Honors Thesis on remote sensing of water quality. She used this project's resources to analyze water samples for estimating total suspended sediments (TSS). Abbie recently accepted a position in the remote sensing division of the Oak Ridge National Laboratory (ORNL).

Shuvashish Roy: Mr. Roy joined this project as a graduate (MS) student in Civil Engineering. He graduated in May 2020 and recently joined the industry as an engineer. He was instrumental for the development of the EFDC 3D hydrodynamic model for part of the Tennessee River.

Syed Tareq: Mr. Tareq joined this project as a graduate (MS) student in Civil Engineering. He also graduated in May 2020 and started pursuing a PhD in Computational Engineering at UTC. He was also involved in the development of the EFDC 3D hydrodynamic model for part of the Tennessee River.

Community and Broader Impacts

The City of Chattanooga, TN, has grown substantially during the last several decades and has become the center of a series of urbanized sub-watersheds. The environmental impacts, especially the quality of surface waters due to this growth, have become a major concern for the sustainable developments of the Greater Chattanooga area. This project, provided with the potential proof of concept of satellite-based remote sensing-integrated water quality modeling capability, would provide a powerful tool to study the impacts of land use and land cover change on the surface water quality in the watersheds of southeast Tennessee. The obtained results of this project would also provide a unique approach to study surface water quality in other areas in the United States and the rest of the world as well.

This research advances BGE, College of Art and Sciences, and University Strategic Plan goals to involve students in meaningful experiential learning and to be an engaged metropolitan university conducting innovative research of local, regional, and national interests. This research also advances UTC's goal of building capacity and expertise in GIS and remote sensing. This project supports and contributes significantly to advance the SimCenter's mission in the environment research thrust by developing new innovative research at UTC on surface water quality modeling and simulation.

Scholarly Products

Publications:

Manuscripts Published

- Hossain, A. Mathias, C. and Blanton, R., 2021, Remote Sensing of Turbidity in the Tennessee River Using Landsat 8 Satellite, Remote Sensing, 2021, 13, 3785. https://doi.org/10.3390/rs13183785.

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

- Dey,P., Roy, S., Bathi, J., Mishra, A., Leasi, F., and Hossain, A., 2021, Parameter Sensitivity Analysis of the HSPF Model on a Pervious Landcover Dominated Watershed, Proceedings of EWRI Congress 2021, 561-574, https://ascelibrary.org/doi/abs/10.1061/9780784483466.051.

Manuscripts in Preparation (All data processing and analyses have been completed. Manuscript is in draft form)

- Hossain, A., Mathias, C., and Blanton, R., Exploring the potential of Sentinel - 2 satellite imagery for quantitative surface water quality estimation in Southeast Tennessee. The manuscript is under preparation and to be submitted to Remote Sensing of the Environment.

- Hossain, A., Blanton, R., and Mathias, C., Quantitative Remote Sensing of Surface Water Quality in Southeast Tennessee Utilizing Planet Dove Imagery. The manuscript is under preparation and to be submitted to Remote Sensing.

External Conferences:

- Faxon, A., Hossain, A., Mies, J., and Shirmeen, T., 2022, Studying Suspended Sediment Concentrations in the South Chickamauga Creek using Satellite Imagery and Numeric Modeling, ASPRS 2022 Annual Conference, Virtual, March 21-25, 2022.

- Faxon, A., Hossain, A., Mies, J., and Shirmeen, T., Studying Suspended Sediment Concentrations in the South Chickamauga Creek of Chattanooga, TN using Satellite

Imagery, Digital Image Processing, and Numeric Modeling. NCUR 2022 @Home on April 4-8, 2022.

- Hossain, A., and Mathias, C., 2021, Remote Sensing of Water Quality in the Tennessee River Using Sentinel-2 Imagery, GSA Southeastern Section - 70th Annual Meeting – 2021, April 1-2, 2021, Online Meeting. GSA Abstract #362338.

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

- Hossain, A., Blanton, R., and Mathias, C., 2019, Surface Water Quality Monitoring Using Remote Sensing Technology in Chattanooga. SWPBA 46th Annual Meeting in Chattanooga, TN October 14th to 17th, 2019.

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

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

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

Presentations at UTC:

- Hossain, A. and Mathias, C., 2021, Remote Sensing of Water Quality Using Planet Dove Imagery, 6th Annual UTC Research Dialogue, April 12-15, 2021. The University of Tennessee at Chattanooga.

- Mathias, C. and Hossain, A., 2020, Bathymetric digital elevation model for the Tennessee River. 5th Annual UTC Research Dialogue, April 14-15, 2020. The University of Tennessee at Chattanooga. Conference canceled due to COVID-19 situation.

- Hossain, A., Blanton, R., and Mathias, C., 2020, Surface water quality estimation in Southeast Tennessee using Sentinel - 2 satellite imagery. 5th Annual UTC Research Dialogue, April 14-15, 2020. The University of Tennessee at Chattanooga. Conference canceled due to COVID-19 situation.

Inventions or Other Intellectual Property

The proposed remote sensing-integrated numerical water quality model is a new and unique approach of surface water quality study. Upon publishing the research, we will try to develop partnership with commercial satellite companies like Planet Laboratory Inc. to estimate satellite observed water quality data at regular intervals and/or as needed using the developed models. I am interested in learning more about the invention disclosure/commercialization process.

Research Outreach & Collaboration

This project helped us to continue our current research collaboration with the National Center for Computational Hydroscience and Engineering (NCCHE) at the University of Mississippi as this study generated additional proof of concepts of the remote sensing-integrated water quality modeling in the Tennessee River.

This study can be considered as a follow-up and complementary to UTC's "Urban Streams Project" (1998–2000) as it is monitoring selected streams in the Chattanooga area (Tennessee—Georgia). The obtained research results provide valuable information on the health of the city's stream ecosystems. Such information can be utilized by the city of Chattanooga, the Tennessee Department of Environment and Conservation (TDEC), the Tennessee Wildlife Resources Agency (TWRA), the Tennessee Aquarium Conservation Institute, and the Tennessee Valley Authority. Currently we have started a research project with TWRA. Recently, we also submitted a research proposal to the city of Chattanooga related to this project. We also had research collaboration meetings with TDEC to synchronize their field data collection program with satellite image acquisition.

EXTERNAL FUNDING

Contracts/Awards Received

- Urban Streams Restoration Project. Agency: Tennessee Wildlife Resources Agency. Duration: 07/01/2020–06/30/2023. Amount: $36,000. Role: Co-Principal Investigator (Principal Investigator: Mark Schorr).

Proposal Submissions

- Urban Streams Restoration Project: Measuring the Efficacy of Habitat Mitigation/Restoration Efforts on Chattanooga Area Streams: Citico Creek, Friar Branch, and Mountain Creek. Agency: City of Chattanooga. Duration: 01/01/2020–08/31/2022. Amount: $43,869. Role: Co-Principal Investigator (Principal Investigator: Mark Schorr). Pending.

- Integration of Remote Sensing Technology with Hydrodynamic Models for Surface Water Quality Monitoring in Southeast Tennessee. Agency: USGS through Tennessee Water Resources Research Center (TNWRRC). Duration: March 1, 2020–February 28,

2021. Total amount: $24,976 (Federal) and $50,390 (Non-federal). Role: Principal Investigator. Not funded.

- Integration of remote sensing technology and numerical model for water quality study in Mississippi Sound. Agency: The Mississippi Based RESTORE Act Center of Excellence (MBRACE) at the University of Southern Mississippi. Duration: 01/01/2020–12/31/2021. Total amount: $87, 88. This proposal was submitted by The University of Mississippi in collaboration with The University of Tennessee at Chattanooga (UTC). Role: Co-Principal Investigator [UTC Principal Investigator]. Not Funded.

Sponsored Program Capacity Building Activities

Attended webinar organized by the Tennessee Water Resources Research Center (TNWRRC) at the University of Tennessee at Knoxville after getting invited to submit a proposal to the National Institutes for Water Resources at the U. S. Geological Survey.

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 follow up my CEACSE grant with the following work within next three years:

- Publish 3–4 journal articles based on the obtained results—next one year.
- Extend the work into the recently awarded project with Tennessee Wildlife Resources Agency (TWRA) and the pending project with the city of Chattanooga—next three years.
- Submit proposals to NSF, NASA, and USGS (TNWRRC)—next two years.
- Develop a web-based modeling platform at GERSLab to apply remote sensing-integrated models to estimate water quality parameters for the Tennessee River and the adjacent water bodies—two to three years.

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

I will continue working toward my current research collaboration with the National Center for Computational Hydroscience and Engineering (NCCHE) at the University of Mississippi to support them seeking research funds from the Mississippi Based RESTORE Act Center of Excellence (MBRACE) at the University of Southern Mississippi.

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

The data and research results obtained from this project will be used for the Smart River Project, which is a collaborative effort between the SimCenter and the National Center for Computational Hydroscience and Engineering (NCCHE) at the University of Mississippi through the NSF Project entitled "CC*Compute: A Cost-Effective, 2,048-core InfiniBand Cluster at UTC for Campus Research and Education".

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

The barriers that I anticipate facing in order to reach the next goals are the availability of external research funds and heavy teaching loads during regular semesters.

FINANCIAL ACCOUNTING

The total approved budget of the project was $96,488.00. By June 30th, 2020, the actual amount spent on the fund is $78,620.94. Due to the COVID-19 pandemic, it was not possible to spend all the funds allocated for students' support and travel. There were also unspent funds for publication fees. From the remaining balance ($17,867.06), $14,200.00 has been approved to carryover for the 2021 and 2022 fiscal years for students' support, travel, and publication fees.

Fiscal Year 2022 Final Project Report

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

Hamdy Ibrahim, Lead PI

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

Project Title: “Corrosion modeling of magnesium-based fixation hardware for mandibular reconstruction surgeries”

Date Submitted: 09/23/2022

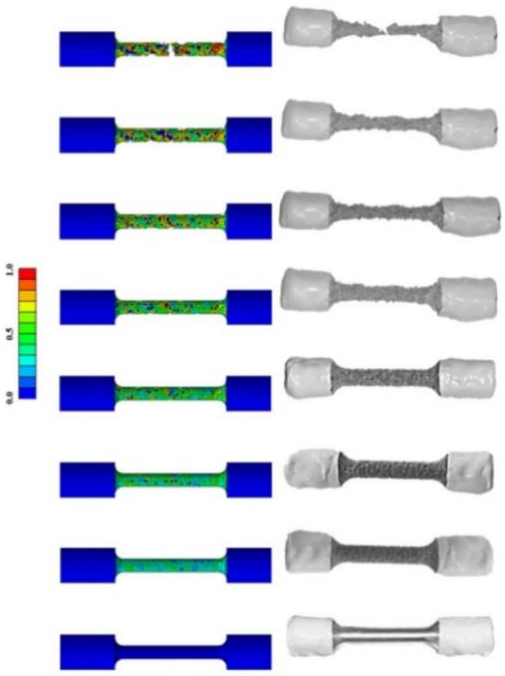
Award Start—End Date: July 1, 2019–June 30, 2021

Non-Technical Summary:

The long-term objective of this research is to develop biodegradable (nonpermanent) magnesium-based bone implants with suitable mechanical, physical, and biological properties to address the drawbacks of the currently-in-use permanent bone implants. This funded project succeeded in developing a subroutine and a model to predict the corrosion rate of biodegradable magnesium-based alloys for their biomedical applications. This model was calibrated by conducting a series of tests in conditions simulating the body’s environment. The findings of this study increased the knowledge on the biomechanical performance of biodegradable magnesium-based materials. The project has also enhanced the infrastructure for research and education by increasing the level of current activity in the area of biomaterials. Four students (2 graduate and 2 undergraduate) were trained through this project in corrosion modeling, experimental corrosion testing, microstructural characterization, and mechanical testing. Several corrosion testing tools and devices were purchased from this project that will be available, for the first time, to faculty and students at UTC to test the corrosion characteristics of metals and alloys.

PROJECT TITLE: Corrosion modeling of magnesium-based fixation hardware for mandibular reconstruction surgeries

Technology Area of Interest: Health and Biological Systems + Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
• Developing the subroutine (code) that can simulate the corrosion behavior of Mg alloys using the continuum damage mechanics theory. • Calibrating and validating the subroutine parameters using in vitro immersion test results.	A code was developed based on the continuum damage mechanics theory for the pitting corrosion, compressive stress corrosion, and tension stress corrosion to assess the overall damage as corrosion proceeds. The model was calibrated by conducting a series of tests in conditions simulating the body's environment. The results of this work resulted in the submission of 2 journal papers, 1 conference presentation and 2 NSF proposals.
RESULTS	**OTHER INFO**
	**Budget and Schedule** Total Budget: $99,905.99 Actual Used: $99,905.00 Balance: $1.00 Total period of performance is 12 months. Task 1: Months 1–6 Task 2: Months 3–6 Task 3: Months 6–12 Task 3: Months 8–12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication • External and internal conference presentation **Organization Information** Dept. 2502, 615 McCallie Avenue, Chattanooga, TN 37403, Ph: 423-425-4718 Email: Hamdy-Ibrahim@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Modeling the corrosion behavior of Mg-based material in pitting corrosion, compressive stress corrosion, and tension stress corrosion.	A VUMAT in the finite element solver "Abaqus/Explicit" was generated. The model was developed based on the continuum damage mechanics theory.
Performing a series of in vitro immersion tests to calibrate and validate the developed model.	The in vitro immersion test was conducted on a series of coupons, compression cylindrical specimens, and tension dog-bone specimens. The specimens were tested in simulated body fluid under permanent compressive stresses during the duration of the in vitro immersion test (3 months).
Using the developed corrosion modeling VUMAT subroutine with a previously developed 3D model to simulate a mandibular reconstruction surgery.	This was a secondary objective in the project, and due to the limitation in resources and time we decided to keep it for future research work.

Challenges & Strategies Used to Address / Overcome:

The main challenge we faced was the lockdown due to the COVID-19 pandemic, which resulted in a delay with the corrosion testing work. We managed to perform most of the needed tests, especially the immersion test work. However, we conducted most of the needed tests during the one-year extension period.

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

N/A

IMPACT & OUTCOMES

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

The PIs gained a fundamental understanding of corrosion modeling of magnesium alloys as a new class of regenerative skeletal fixation devices using continuum damage mechanics. The project also enhanced the available infrastructure for the PIs and other researchers at UTC to conduct future research on the corrosion of metals and other activity in the area of biodegradable materials. Finally, the pilot data of this project and the provided support helped the PIs to prepare and submit two NSF proposals and to submit two journal papers.

Students Impacted

- **Moataz Abdalla**, graduate student: He was completely funded and led the students' effort in this project for one year. He is expected to graduate spring 2021.
- **Austin Sims**, graduate student: He was partially funded in this project. He is expected to graduate fall 2020.
- **Alexander Joplin**, undergraduate student: He was partially funded in this project during spring and summer 2020.
- **Clay Jones**, undergraduate student: He was partially funded in this project during spring 2020.

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. Two graduate students and two undergraduate students were involved in this project. They learned about the technical aspects of the project in addition to giving presentations about their work.

Scholarly Products

Publications:

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

External Conferences:

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

Presentations at UTC:

N/A

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

- **Ibrahim, H.**, “Treating Bone Trauma Using ResorbFix”, I-Corps Teams, submitted to the National Science Foundation (NSF), 2020. *Requested amount*: **$50,000**. *Status*: **Awarded**.
- **Ibrahim, H.**, Mahtabi, M., Danquah, M., Elliot, T., Palchoudhury, S., Elliot, L. & Panagiotou, E. “Acquisition of a customized metal additive manufacturing system for multidisciplinary research activities”, Major Research Instrumentation Program: (MRI), submitted to the National Science Foundation (NSF), 2020. *Requested amount*: **$261,500**. *Status*: **Not Funded**.

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 am planning to identify some potential collaborators with medical backgrounds (e.g., Erlanger or other universities) to expand the scope of my research to include more interdisciplinary activities.

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 2022 Final Project Report

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

Loren Hayes, Lead PI

Co-PI(s): Jin Wang
Other Personnel: Craig Tanis (former co-PI), Elizabeth Pope (student), Evan Suggs (student), Braxton Anzalone (student), Azad Hossain (unfunded faculty)

Project Title: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models

Date Submitted: 2019

Award Start—End Date: July 1, 2020–June 30, 2021 (extended to June 2022)

Non-Technical Summary:

A fundamental goal of biology is to understand the evolution of animal social systems. Comparative studies have failed to account for intraspecific variation in social organization (e.g., a species may live in groups or alone in different populations). Accounting for intraspecific variation in comparative studies is critical because the ability to change social organization may improve species resilience in the face of climate change. We aimed to: (i) build a dataset on mammalian social organization that accounts for intraspecific variation and (ii) conduct a preliminary analysis to determine the impact of rainfall and temperature trends on artiodactyl social evolution. We focused on artiodactyls because Lead PI Hayes has completed manual data collection for this order. We conducted a semantic analysis of the literature, applying machine learning techniques to improve the consistency and speed of data collection (aim 1). After a co-PI left the university, we began a mathematical modeling project to predict conditions favoring variable social organization (revised aim 2). The latter project involved collaborations across three departments (biology, geology, math), building on the SimCenter mission to foster cross-disciplinary collaborations. The funding also promoted collaborations with colleagues at research institute in Strasbourg, France, building international recognition.

The project directly supported three students, one each in biology, geology, and computer science. Tanis supervised a website project involving four unfunded engineering students and Hayes worked with a French graduate student on a related project. One student (Suggs) produced a poster at a scientific meeting. The project was successful in generating datasets on artiodactyl social organization and life span as well as rainfall specific to artiodacytl entries in our dataset. We will use the results of this study to strengthen a National Science Foundation proposal to conduct a comparative analysis of how climatic variation influences the evolution of mammalian (~5500 species) social organization.

PROJECT TITLE: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models

Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
The main goal was to contribute to a dataset on mammalian social organization. This dataset would be used to answer questions about the evolution of variable social organization. Tasks included: • Collect data social organization and life history dataset for artiodactyls • Develop plan for mathematical modeling • Extract rainfall data from online data sources • Develop search tool based on machine learning	We accomplished the following: • Data on artiodactyl group sizes collected for ~200 populations. • Life history data for ~20 species collected from the literature. We conducted a statistical analysis to determine if data from the primary literature align with commonly used online databases (key for quality check prior to NSF submission). • Wang developed a mathematical model using data provided by Pope. • Azad Hossain and student extracted rainfall data for >10 years from the online database (CRU). This project will be completed summer 2021. Suggs presented data on his machine learning project at a national meeting.
RESULTS	**OTHER INFO**
The are no major 'results'. However, data collected during the period of funding will contribute to a NSF proposal. Critically, we compiled rainfall data, evaluated the quality of life history datasets, and are building a predictive model needed to justify some of the questions. Insight from the project supported a paper submission on a related project and the development of a new student project. Hossain, Wang, and Hayes submitted a proposal to ORCD.	Due to a change in personnel and the COVID-19 pandemic, the project has been extended until June 2022. **Budget and Schedule** Total Budget: $98,662.00 Actual Used: $98,665.46 Balance: $555.45 Total period of performance is 12 months. **Deliverables** • Quarterly reports describing progress and challenges • Final report detailing results, financials, and future work • Olivier, C. A., Jaeggi, A. V., Hayes, L. D., & Schradin, C. (2022). Revisiting the components of Macroscelidea social systems: Evidence for variable social organization, including pair-living, but not for a monogamous mating system. Ethology, 128(5), 383-394. • UTC Research Dialogues presentation • External conference presentation (Evan Suggs) **Organization Information** Departments of Biology, Geology, and Environmental Science and Department of Mathematics, University of Tennessee at Chattanooga

ACCOMPLISHMENTS & OUTCOMES

Overview:

A fundamental goal of biology is to understand the evolution of animal social systems. Most comparative studies aimed at explaining the diversification of bird and mammal social systems have failed to account for intraspecific variation, even though there is considerable evidence that many species have more than one form of social organization (e.g., can live in groups and alone at different times of the year or in different populations). Building datasets that account for intraspecific variation is essential for accurate evolutionary analyses and the determination of how climatic factors influence the ways that animals live. Proposal aims are: i) build a high-quality dataset on intraspecific variation in mammalian social organization and ii) conduct a preliminary analysis to determine the impact of historical trends in rainfall and temperature on the social organization of the mammalian order Artiodactyla. The co-PIs (lead PI: biology, geology and environmental science; Co-PI: computer science) and students developed machine-learning techniques to improve the quality and speed at which datasets can be built and develop preliminary computational models that attempt to correlate climate change and mammalian social organization. They also collected vital data on social organization, life history, and rainfall for a NSF proposal and developed a mathematical model.

Intellectual Merits:

Previous comparative studies of mammalian social evolution relied on faulty assumptions. The lead PI's ongoing research on intraspecific variation in social systems has challenged the conclusions of these studies and has the potential to transform social evolution theory. However, progress has been slowed by the laborious task of large database searches and lengthy data collection from published papers. Moreover, we need a predictive framework based on preliminary analyses of a subset of data to justify an expanded study on all mammals. Automated searches developed in the proposed study will be used to complete and maintain the lead PI's dataset on mammals and have broad application to comparative studies of animal social systems. Critically, a conceptual framework will emerge from the preliminary analysis on artiodactyls, strengthening an NSF proposal aimed at determining how climatic variation influences intraspecific variation in mammalian social systems. This research is timely for two reasons. First, recent advances in comparative methods now permit researchers to account for intraspecific variation. Second, understanding intraspecific variation is crucial to predicting how different species may respond to rapidly changing environments. The collaboration has already generated some funding to develop search code necessary to achieve the proposal aims.

Outcomes:

(1) Completed a dataset on artiodactyl social organization, adding group-size data and life history, (2) started collecting rainfall data to populate the social organization dataset, (3) developed a mathematical model to predict how rainfall influences artiodactyl social organization, (4) established cross-disciplinary collaborations, (5) strengthened an international collaboration with a colleague in France, (6) presented results at UTC, a regional meeting, and to an international audience, and (7) connected CEACSE funded research to Hayes' NSF IRES program. A related paper was published in *Ethology*. Hayes and Wang are now collaborating with Hossain on a ODRD proposal with colleagues at NOAA.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Building an artiodactyl dataset	Added information on group size, moved species level information to populations, added life history data from primary literature.
Life history analysis	Compared data from primary literature to online database, conducted statistical analysis.
Rainfall dataset	Using GPS locations from artiodactyl dataset, we extracted rainfall data (1900–present) from CRU dataset.
NSF proposal	Submitted an NSF proposal in summer 2020. The proposal built on aims of this project.
Connected CEACSE funded project to Hayes' NSF IRES grant	A student working on a related project (mating systems) collaborated with Schradin (France). The student was funded by Hayes' NSF IRES program. A graduate student was funded in spring 2022 (by CEACSE) and now is working in Chile on NSF funding.
Build student capacity	Trained students in computer science, biology, geology; also worked with students in different countries on related projects. Former co-PI Tanis supervised 4 engineering students working on a website and a graduate student funded by the project.

Challenges & Strategies Used to Address / Overcome:

1. Co-PI Tanis left UTC after the fall 2020. Wang was added as a co-PI, formalizing his role in the project. He had contributed to a prior NSF grant proposal submission. The change also freed up funds to support a geology student working with Hossain.
2. COVID-19 impacted everyone. All activities were moved online. However, this opened some possibilities, including the FINE Seminar (see below) and weekly international lab group meetings with Schradin.

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

The machine learning project did not progress as planned. Tanis left UTC and his student (Suggs) moved on to another project. However, this opened up new avenues of research with colleagues in math and geology.

Pope left the M.S. program after one year. Losing her created some challenges (lost project memory, continuity). However, Hayes continued to communicate with her about her work and she has shared information freely with Hayes and collaborators. We used the remaining CEACSE funding to support a new student (Logan Platt).

IMPACT & OUTCOMES

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

Funding permitted the development of a collaboration between Hayes and Schradin (France). The work will ultimately generate numerous papers on mammalian social evolution. Time freed from teaching allowed Hayes to co-organize an international seminar series and hold Thursday morning meetings with his students and members of Schradin's lab group.

Hayes was promoted to Full Professor.

Hossain was promoted to Associate Professor.

Students Impacted

Elizabeth Pope – environmental science, M.S.: Pope analyzed life history data and contributed to a UTC Research Dialogues poster. She did an excellent job with the analysis and trained several other students. She left the M.S. program to pursue other goals.

Evan Suggs – computer science, M.S.: Suggs worked on machine learning projects and is entering his second year of the M.S. program. He had a change in PI due to the departure of Tanis from UTC.

Braxton Azalone – geology, undergraduate: Azalone is working on a rainfall dataset in summer 2021. He plans to graduate in 2022.

Madison Roberts – biology, undergraduate: Roberts is working with Schradin on a related project and is supported by NSF IRES. She was not funded by CEACSE. She plans to continue her project into fall 2021, leading to an honors thesis.

Madeline Townsend – biology, undergraduate: Townsend worked on a related project (Cetacean social organization) but was not funded by CEACSE. She graduated from UTC in spring 2021.

Logan Platt – ESC, graduate student: Worked with a colleague in Colombia to prepare a large dataset for future collaboration (using R).

Community and Broader Impacts

Hayes' students participate in a remote, international seminar on animal social evolution (Frontiers in Social Evolution, FINE). The seminar series includes 15 talks. CEACSE funded students were able to meet individually with the speakers. In this way, the program has enhanced the education of Hayes' students.

Students working on this project have had opportunities to interact and collaborate with colleagues at multiple institutions outside UTC, including Yale University and University of Strasbourg. Through these activities and FINE, students are building international networks.

Hayes and the other FINE coordinators have developed teaching tools that are broadly accessible. Teaching tools include lecture slides prepared by FINE speakers, reading lists, and a certificate of participation that students can use to earn university credit.

Scholarly Products

Publications:

Olivier, C. A., Jaeggi, A. V., Hayes, L. D., & Schradin, C. (2022). Revisiting the components of Macroscelidea social systems: Evidence for variable social organization, including pair-living, but not for a monogamous mating system. *Ethology*, *128*(5), 383-394.

External Conferences:

- Suggs, E.D. 2019. Meta-textual analysis of biological research. ACM meeting, Gatlinburg, TN.
- Miles, M. Variable social organization is ubiquitous in Artiodactyla and probably evolved from pair-living ancestors. Summer 2020, presentation to Hayes, Schradin (France), and Fernandez-Duque (Yale) lab groups.

Presentations at UTC:

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

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

Carsten Schradin, IPHC, France. Schradin and I are working together on the mammalian social evolution project. We have submitted 3–4 papers on this topic and plan to continue collaborating into the future. Schradin is also participating in my NSF IRES program as a mentor to Madison Roberts (UTC student). Roberts is working on a related study of mammalian mating systems.

Azad Hossain, Geology, UTC. We are working on a rainfall dataset. In summer 2021, his student used GIS software extract rainfall data based on GPS locations associated with artiodactyl populations in our dataset. This information will be used to inform a NSF proposal.

Jin Wang, Math, UTC. Wang is building a mathematical model to assess how variation in rainfall influences variation in social organization within populations. This will inform a NSF proposal and potentially open the door for new questions.

Frontiers in Social Evolution Seminar (FINE). Schradin and I co-coordinate an international, remote seminar on animal social evolution with Dr. Eduardo Fernandez-Duque (Yale). The FINE is attended regularly by 100 people worldwide. The third series will begin in September 2021. This activity will become part of a broader impacts section of an NSF proposal. https://www.socialevolutionseminar.com. Interestingly, a student taking Biology 1130 with Hayes worked with Fernandez-Duque in Argentina, highlighting the benefits of networks developed in this project.

EXTERNAL FUNDING

Proposal Submissions

NSF IOS, Comparative and computational analyses of climatic and life history drivers of variable social organization in mammals. Submitted in summer 2020, declined. (Hayes, Tanis, and Wang co-PIs)

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

- Consultations with NSF IRES program officer.
- Managed my NSF IRES grant.

WHAT'S NEXT FOR THIS RESEARCH?

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

I plan to continue my collaboration with Schradin, Wang, and Hossain for the foreseeable future. We plan to write grants to support related projects. The project will likely generate papers for the next 5–10 years.

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

Wang: Mathematical modeling of how rainfall influences social organization.

Hossain: Geological significance of environmental variation in mammalian populations.

Schradin: Social evolution of mammals.

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

Students in my IRES program interacted with international collaborators in my CEACSE project, creating new networking opportunities.

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

Steady progress towards the overall project goals will require NSF funding. My first proposal received some decent reviews but was deemed not competitive. Data generated by the CEACSE could help to improve the proposal quality. The main challenge will be time. It is difficult to complete all these tasks, including writing a good grant proposal, when my teaching load is 6–9 hours per week.

I have established a collaboration with a colleague at UT-Austin. We plan to discuss the proposal in the coming months.

Collaborations with Wang and Hossain as well as colleagues at NOAA could build capacity.

FINANCIAL ACCOUNTING

Due to a change in personnel (Tanis left UTC), some funds were not spent. Some of the funds were reallocated to Wang and a Geology student. We used most of these funds to support a graduate student in spring 2022.

Fiscal Year 2022 Final Project Report

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

Lead PI – Mina Sartipi

Co-PI(s): Farah Kandah, Osama Osman
Other Personnel: N/A

Project Title: "Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications"

Date Submitted: 09/27/2021

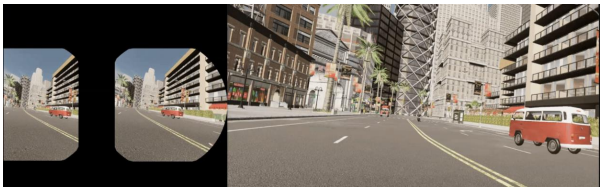
Award Start—End Date: July 1, 2020–June 30, 2022

Non-Technical Summary:

The proposed research includes modeling, simulation, and computational performance analytics and optimization. The proposed research aims to apply Virtual Reality (VR) in a multi-player game setting for a wide spectrum of research applications at the University of Tennessee at Chattanooga (UTC). Specifically, an integrated multidisciplinary human-in-the-loop simulation platform will be developed to enable studying micro-level interactions between multiple heterogeneous road users in a VR multiplayer setting. The research objectives are to: (a) develop an integrated simulator for heterogeneous road users that capitalizes on VR technology; (b) develop a behavioral data collection and visualization tool for the integrated simulator; and (c) demonstrate the capabilities of the integrated platform. The proposed integrated simulation platform facilitates experimental research and training in highly controllable conditions. Additionally, the integrated platform can combine the various advantages of various research methods: pedestrian-in-the-loop simulation for testing of pedestrian behavior in a wide range of applications, driver-in-the-loop simulation for experimental investigation of driver behavior in various scenarios, and data analytics and visualization techniques of behavioral data. The integrated platform adds a high degree of realism since assumptions and mathematical models of road user behaviors will not be the basis of simulation. This platform can also enable subjective feedback (e.g., emotions) of road users in addition to objective parameters (e.g., actual actions). This work can be collaboratively conducted by Principal Investigators (PIs) with extensive and complementary expertise in human factors research, application of gaming in research, data analytics, smart communications and vehicle networks, computer networks, performance optimization, software-defined networks, and game design and production.

PROJECT TITLE: Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications

Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
1. Literature Review 2. Equipment Purchase, Installation, and Configuration 3. Developing an Integrated Heterogeneous Simulator 4. Developing a Behavioral Data Collection and Visualization Interface 5. Developing Use Case for SmartSim 6. Writing Final Report and Planning for Extramural Funding	The team has conducted a comprehensive literature review and identified similar work for potential knowledge transfer and to help with the work proposed herein. The team purchased all the necessary equipment, including a driving simulator and a head mount display with the required accessories. The team purchased a computer to be dedicated to the HMD. Finally, the team worked on the development and integration process.
RESULTS	**OTHER INFO**
	**Budget and Schedule** Total Budget: $99,998.00 Actual Used: $89,641.78 Balance: $10,356.22 Total period of performance is 12 months. Task 1: Months 1-2 Task 2: Months 1-4 Task 3: Months 5-14 Task 4: Months 7-12 Task 5: Months 11-15 Task 6: Months 15-18 **Deliverables** • Quarterly reports describing progress, challenges, and future plans. • Final report describing progress, challenges, and future plans. **Organization Information** University of Tennessee at Chattanooga, P: 423-425-5336; mina-sartipi@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Literature Survey Results:

Recently, Virtual Reality (VR) is gaining enormous research focus, especially in traffic simulation and visualization. However, the advantage of VR is not fully exploited when using flat screens and desktop simulators. This is because users do not feel they are fully immersed into the simulation environment. One way of surmounting this was with a cave setup where large screens surround the subject at 85-degree angles to the right and left. The disadvantages of this setup are that it requires large spaces, and it is very costly [1]. Another promising solution is the use of Head-Mounted Displays (HMD). The HMD is now affordably available, and its size is smaller compared to cave setup [2]. Further, the advantage of a 360-degree field of view over the flat screen makes virtual reality models feel realistic for users inside the lab [3]. Thus, scholars used this technology to mimic and measure real-life metrics in a virtual environment with different scenarios. Accordingly, such metrics are now possible to be measured accurately with the help of computer simulators. Confirming these findings, Mallaro et al. [4] compared HMD and screen-cave setup and concluded that users with HMD had a near realistic experience compared to their peers with the screen-cave setup.

Methodology:

This research is mainly entitled to study the interaction between vehicles, drivers, and pedestrians through computer simulations. In doing so, the CARLA simulator is used as the study ground. The CARLA Simulator [6] is an open-source simulator and it is developed mainly for Autonomous Vehicle (AV) studies and interaction. CARLA developers can use python to develop and control AV with different sensors. Computer screens are used to simulate the vehicle windows and mirrors. Through CARLA, developers also can simulate pedestrians with their own trace and trajectories. As suggested and concluded by [1], Head Mounted Display (HMD) offers full immersion and stereovision to users for in-street crossing behavior. In addition, [4] stated that users who used HMD were less conservative in their spacing and time between objects and street crossing. Accordingly, and for this reason, Head Mount Display is used to mimic the pedestrian interaction through CARLA and the trajectory of the HMD is projected on CARLA.

CARLA has been built on the open-source graphics game engine, Unreal Engine (UE). The final development package of the CARLA simulator is illustrated in Figure 1. As shown, the package has two separate projects; CARLA and UE. Each project has been developed separately by two separate entities. Then, a link between CARLA and UE was developed by CARLA developers. In CARLA, HMD is not enabled by default. The following steps were designed to enable HMD in CARLA:

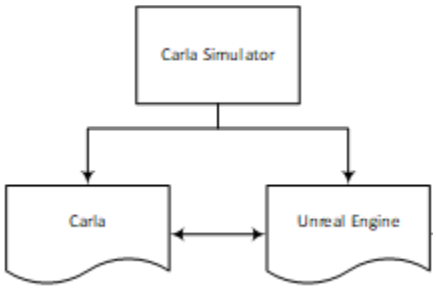


Figure 1: CARLA Simulator Package

Step 1: Getting CARLA and Unreal Engine (UE) Source Code

Considering our final target, which is developing an interaction between a pedestrian (HMD) and vehicle drivers, we needed to enable HMD in CARLA. Since CARLA is built on and uses the Unreal Engine (UE), any development related to simulation should be done on UE. Having said that, since HMD integration is not enabled in a plug-n-play fashion in CARLA, downloading the source code for both CARLA and UE from Github is necessary. The dependencies for Compiling CARLA Simulator (CARLA and UE) needed to be installed afterwards.

Step 2: Enabling HMD in UE and CARLA project

In UE, the pedestrian is modeled as a character with attached movements such as walking and running movements. When loaded inside UE, this character and all the attachments get bound to the character, and they become the pedestrian. Because HMD works as a display, a camera was added and attached to the character mesh through a socket. This is because UE uses cameras to link HMD to any scene (Figure 2). Afterwards, the camera rotation and transformation could be controlled by the HMD movements.

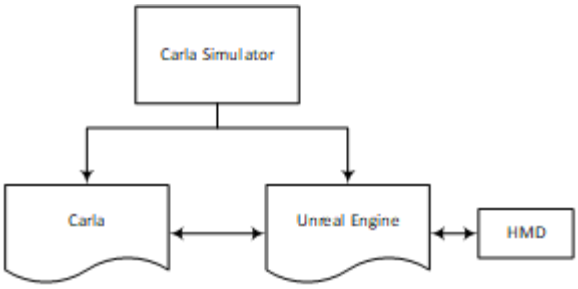


Figure 2: Modification to the CARLA Simulator Package

Step 3: Modifying UE environment and controlling the scene movements

CARLA development was done on the basic-flat mode of UE where the UE scene is only reflected on computer screens. In our case, the Virtual Reality mode is needed for the HMD control. With such control, UE gets the transformation required for the scene from the HMD's movements. At this point, HMD movements handle triggers in UE. Transforming the scene in UE needed to be done manually through UE visual programming.

Step 4: Camera movements and trajectory

Now, the HMD is mounted on a pedestrian and exactly on his face. Also, the camera (pedestrian's face) controls the UE/CARLA scene. In addition, as the pedestrian moves, a trajectory file of the pedestrian is created on the computer hard drive for later research.

Final Output:

Figure 3 shows the result of HMD & CARLA integration. On the left is the HMD view and on the right is the flat screen view. In this scene, a person was wearing the HMD while moving around and rotating their head in all directions. The HMD could smoothly transform the scene to the new virtual view. This integration gives a chance to study the pedestrian-vehicle interaction by implementing a wheel control or a pedestrian-AV interaction.

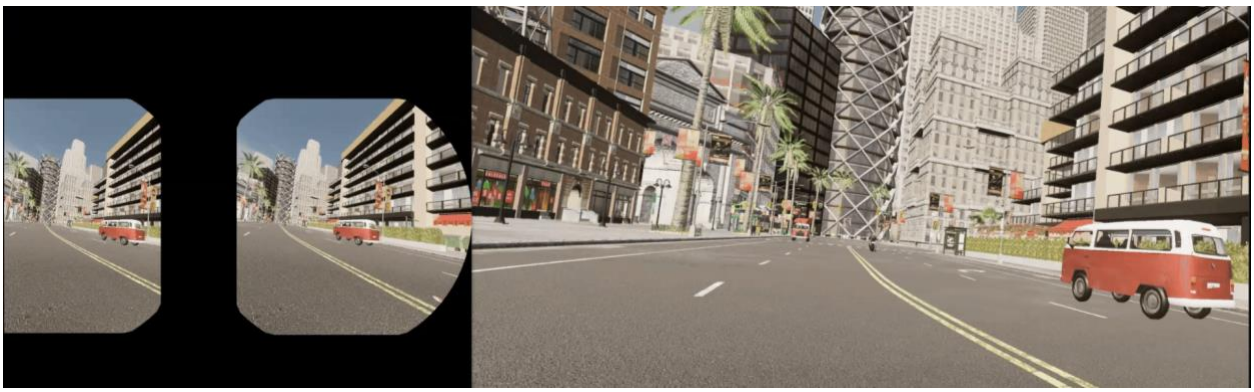


Figure 3: HMD & CARLA Integration Result

References

- Pala, P., V. Cavallo, N. T. Dang, M. A. Granié, S. Schneider, P. Maruhn, and K. Bengler. Is the Street-Crossing Behavior with a Head-Mounted Display Different from That Behavior in a CAVE? A Study among Young Adults and Children. Transportation Research Part F: Traffic Psychology and Behaviour, Vol. 82, No. November 2020, 2021, pp. 15–31. https://doi.org/10.1016/j.trf.2021.07.016.
- Stanney, K., B. D. Lawson, B. Rokers, M. Dennison, C. Fidopiastis, T. Stoffregen, S. Weech, and J. M. Fulvio. Identifying Causes of and Solutions for Cybersickness in Immersive Technology: Reformulation of a Research and Development Agenda. https://doi.org/10.1080/10447318.2020.1828535, Vol. 36, No. 19, 2020, pp. 1783–1803. https://doi.org/10.1080/10447318.2020.1828535.
- Nguyen, A., Z. Yan, and K. Nahrstedt. Your Attention Is Unique: Detecting 360-Degree Video Saliency in Head-Mounted Display for Head Movement Prediction. MM 2018 - Proceedings of the 2018 ACM Multimedia Conference, 2018, pp. 1190–1198. https://doi.org/10.1145/3240508.3240669.
- Mallaro, S., P. Rahimian, E. E. O'Neal, J. M. Plumert, and J. K. Kearney. A Comparison of Head-Mounted Displays vs. Large-Screen Displays for an Interactive Pedestrian Simulator. Proceedings of the ACM Symposium on Virtual Reality Software and

Technology, VRST, Vol. Part F1319, 2017, pp. 0–3. https://doi.org/10.1145/3139131.3139171.
- Chioma Ihemedu-Steinke, Q., R. Erbach, P. Halady, G. Meixner, M. Weber, Q. Ihemedu-Steinke, R. Erbach, P. Halady, M. Weber, and G. Meixner. Virtual Reality Driving Simulator Based on Head-Mounted Displays. 2017, pp. 401–428. https://doi.org/10.1007/978-3-319-49448-7_15.
- Dosovitskiy, A., G. Ros, F. Codevilla, A. Lopez, and V. Koltun. CARLA: An Open Urban Driving Simulator. 2017.

Challenges & Strategies Used to Address / Overcome:

The equipment purchase was severely delayed due to the long purchase order process. However, the team has been working to allocate additional resources to make sure milestones for the current quarter are met.

Additionally, upon the PI's request, the award start date was pushed backwards to January 1st, 2021 instead of July 1st, 2020 due to an inability to hire a student because of COVID-19 travel restrictions.

Additionally, remote work imposed by COVID led to severe delays in the purchase and equipment delivery. Accordingly, the currently set end date of the project is June 2022.

Due to the limited power of the graphics card compared to the required power from Carla, we had to reduce the resolution output from the UE. Otherwise, the HMD movements would experience a very long delay. Even though it still experiences some delays, there is a huge improvement.

Finally, the original PI (Dr. Osman) left UTC in January 2022 and Dr. Mina Sartipi was assigned as the lead PI. The Co-PI, Dr. Farah Kandah, also left UTC in August 2022.

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

N/A

IMPACT & OUTCOMES

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

Nothing to report yet.

Students Impacted

Jewel Rana Palit—supported by the grant as a MS student.

Jibril Babatunde—partially supported by the grant as a MS student.

Faiza Khan—partially supported by the grant as a MS student.

All students are supported by the grant at different stages. All students involved in this project gained experience in simulation technologies and VR development.

Community and Broader Impacts

Computer simulations of pedestrian-vehicle interactions will have significant implications for deploying traffic safety measures in a real-world environment. Aggregated data collected from studying these simulated interactions will serve to guide the DOT and city planning officials when making decisions related to traffic safety conditions. The enabling of HMD in Carla can be used to create simulations in other areas of research as well.

Scholarly Products

Publications:

N/A

External Conferences:

N/A

Presentations at UTC:

N/A

Inventions or Other Intellectual Property

Through simulation and the use of these two platforms, the team created a way to enable real interaction between the driver and the pedestrian that will significantly impact the field in providing awareness and supporting for future safety procedures.

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

- A research statement was submitted to the Tennessee Department of Transportation that builds on the integrated platform being developed in this project.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

- NSF CAREER Workshop. Attended by PI Osama A. Osman.

WHAT'S NEXT FOR THIS RESEARCH?

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

Our plan is to pursue grants from NSF and TDOT to showcase benefits of the integrated platform.

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

NSF and TDOT. The team has already started working with TDOT to identify areas of research that could benefit from this work.

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?

Developing the integration is a challenging process. We communicated with the simulator developers and other researchers to get any required input. The purchase of the equipment was severely delayed due to COVID and hiring a graduate student was a more challenging process due to the same reason.

FINANCIAL ACCOUNTING

Remaining is $10,356.22, which was not used and will be returned to the award office.

Fiscal Year 2022 Final Project Report

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

Stephanie DeVries, Lead PI

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

Project Title: "A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers"

Date Submitted: 09/02/2022

Award Start—End Date: July 1, 2021–June 30, 2022

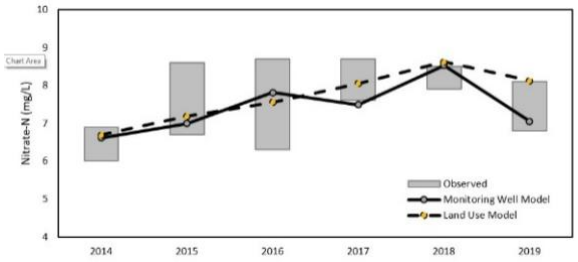
Non-Technical Summary:

The original objective of this project was to evaluate a novel method for digitizing a homogeneous glacial aquifer for 3-dimensional groundwater flow modeling. The model is based on a statistical tool called Thiessen Polygons and can be produced quickly using data reported on well construction reports. More traditional methods of subsurface digitization include statistical models or development of a geologic framework model, which require significantly more expertise and time, which makes groundwater flow modeling cost-prohibitive for some applications. This project aimed to demonstrate that the Thiessen Polygon method yielded statistically comparable results when incorporated into a 3D groundwater flow model.

The original goals of this project were not met largely due to technical difficulties that arose in the development of the geologic framework model using RockWorks. I am still working to resolve that issue and proceed with the work planned. In the meantime, I opted to change the direction of this project to ensure that a measurable outcome would still be achieved in the timeline provided. The revised project goal was to create a stand-alone program written in Python that used output data from a groundwater flow model and historical land-use data to estimate the annual mean nitrate-nitrogen (NO3-) concentration at a pumping well in a well-oxygenated glacial aquifer. This objective has been met and the calculator has been validated against a spreadsheet-based version that has previously been demonstrated to predict nitrate concentration within 5% of observed median values. A manuscript featuring this model is complete and will be submitted to the Environmental Modeling and Software in September 2022.

PROJECT TITLE: A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers

Technology Area of Interest: Environmental Sustainability and Climate Systems

TECHNICAL APPROACH	OUTCOMES
• Develop a 3D geologic framework model of subsurface in Rockworks 3D. • Develop a geostatistical model of subsurface with SGeMS. • Run groundwater flow and particle transport simulations using MODFLOW and MODPATH codes and perform a statistical comparison of capture zones delineated by 3D geologic framework model, geostatistical model, and novel Thiessen Polygon model of subsurface. • Develop a spreadsheet model to estimate nitrate concentrations at a pumping well as a function of land use and travel time inside MODPATH-delineated capture zone. • Develop a Python model to perform the same calculations as the above-referenced spreadsheet. Calculations based on gridded recharge data sets, USDA CropScape data (ASCII), a lookup-table, and travel-time/capture zone (ASCII).	• Develop a 3D geologic framework model of subsurface in Rockworks 3D. • Develop a geostatistical model of subsurface with SGeMS. • Run groundwater flow and particle transport simulations using MODFLOW and MODPATH codes and perform a statistical comparison of capture zones delineated by 3D geologic framework model, geostatistical model, and novel Thiessen Polygon model of subsurface. • Develop a spreadsheet model to estimate nitrate concentrations at a pumping well as a function of land use and travel time inside MODPATH-delineated capture zone. • Develop a C++ model to perform the same calculations as the above-referenced spreadsheet. Calculations based on user-provided recharge, USDA CropScape data (ASCII), a lookup-table, and travel-time/capture zone (ASCII).
RESULTS	**OTHER INFO**
• Spreadsheet model of mean annual nitrate concentration at municipal fit to observed data within 5% (see Figure below)  • Python model estimated nitrate concentration for 2019 at 8.68 mg/L vs. 8.43 mg/L calculated by spreadsheet, which is within the expected margin of error based on differences in the way area and recharge are entered into each model. A graphic of	**Budget and Schedule** Total Budget: $24,981.00 Actual Used: $20,707.28 Balance: $4,273.72 **Deliverables** *indicates undergraduate student author • **Manuscript in Preparation:** DeVries, S., *Hooten, W.G., *Mollica, M. "A model for estimating nitrate in high-capacity wells as function of land use and time-of-travel capture zones in well-oxygenated sand and gravel aquifers." • **Technical Report:** DeVries, S., Bradbury, K., and Cardiff, M. (2022). "A Groundwater Flow Model for Waupaca, WI." Wisconsin Geological Survey and

the model output in terms of mg NO3/grid cell is shown below.	Natural History Survey Technical Report. 007, 88 p., https://doi.org/10.54915/xdis1726. • **Conference Presentation:** DeVries, S., "A modeling tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." GSA NC/SE Joint Sectional Meeting, Cincinnati, OH, April 7–8, 2022. • **Poster Presentation:** DeVries, S.L., *Hooten, W. (2021). A C++ tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." UTC Scholar ReSEARCH Dialogues. • **Poster Presentation:** DeVries, S.L., *Hooten, W. (2020). A C++ tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." Fall Meeting of the American Geophysical Union. • **Invited Lecture:** DeVries, S., "A C++ model for estimating the concentration of nitrate at a municipal well in central Wisconsin." Presented to the Wisconsin Nitrate Task Force on August 21, 2020. • **Invited Lecture:** DeVries, S., "Modeling for decision making: a case study in Waupaca, WI." The City of Waupaca Meeting of the Common Council, Waupaca, WI, May 2019.

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop a Geologic Framework Model for Waupaca, WI, well capture zone	Borehole database and 3D framework model successfully constructed. Conversion of model to input for groundwater flow model is incomplete/pending.
Develop a statistical model of subsurface for Waupaca, WI, well capture zone	Pending
Run groundwater simulations to compare flowpaths and capture zones simulated using geologic framework model, statistical model, and Thiessen-polygon model.	Pending
Develop a spreadsheet-based model that estimates well nitrate concentration as a function of historical land use, annual recharge, and groundwater flow.	Model successfully created. Model predictions are within 5% of observed annual range of nitrate concentrations for two wells in years 2014-2021.
Convert spreadsheet-based nitrate model into a standalone python executable program that requires the following user input: recharge (inches/year), size of gridcell (m), land use codes for relevant time frame input as ASCII files, travel time to well input as an ASCII file, and a lookup table referencing nitrate losses from different land uses.	Program successfully created and tested against earlier spreadsheet models. Simulations run for model years 2014 to 2021 are within 10% of the observed nitrate concentrations and capture annual trends well. The model was used to demonstrate the impacts of different crop rotations on annual nitrate concentrations in a study well.
Develop a Geologic Framework Model for Waupaca, WI, well capture zone	Borehole database and 3D framework model successfully constructed. Conversion of model to input for groundwater flow model is in progress.

Challenges & Strategies Used to Address / Overcome:

The primary barriers encountered during this project were a) getting a late start due to the time-lapse between the onset of the project and the acquisition of necessary computer equipment, b) identifying reliable student researchers, and c) COVID-related issues. The first issue was noted in the mid-project review. Although most of the computers and necessary software were obtained in December 2019, that left just over half of the project period remaining. As new faculty, I sought recommendations from my colleagues for a student capable of aiding in this project. The student hired, based on those recommendations was excited about the project but in reflection, appears to have overestimated their ability to dedicate the time necessary to this project. By the time this became apparent, it was early March and COVID-19 restrictions made it difficult to identify an alternative. At that point, I decided that the best short-term course of action was to proceed on a different, but related project that could be executed in the remaining

time frame by a competent programmer. I reached out to Dr. Anthony Skjellum in March 2020 and hired a student programmer based on his recommendation. The student was highly productive and has worked steadily to complete the C++ model by June 2022.

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

Due to technical and personnel issues, the initial concept was not tested and there are no outcomes related to that concept to evaluate at this time.

IMPACT & OUTCOMES

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

This project will have a long-term and positive impact on the career of the PI. Dr. DeVries is an early-career scientist and the product of this research, a program that models nitrate input to municipal water supplies as a function of land-use and groundwater flow, has practical application in Wisconsin, Minnesota, Michigan, and adjacent areas where nitrate pollution is a major concern affecting the quality of water obtained from unconfined glacial aquifers. The PI published a technical report with a state agency to showcase the conceptual model and framework for the nitrate calculator that was supported by this grant. The C++ model has been presented at national and regional conferences, and the PI has been invited to speak about this model twice. A manuscript featuring the current version of this model is pending and expected to be published in Environmental Software and Modelling by the end of 2022.

The presentations, publications, and student mentorship opportunities afforded by this project will be presented as evidence of the PIs excellence in research and scholarly activities and are expected to have a positive impact on the PI's faculty career and potential to be awarded tenure. Moreover, these accomplishments will improve the PI's visibility in the scientific community and may create new opportunities for research collaboration.

Students Impacted

Gavin Hasty, geology ('21). Developed skill using Rockworks to prepare borehole logs and develop a 3D geologic model. This software is widely used in geologic research and consulting, and the student will benefit from this experience in his professional future.

William (Garrett) Hooten, computer science ('22). Programmed a stand-alone program that calculates the concentration of a contaminant well water as a function of land use using input data from USDA CropScape and a 3D groundwater flow model. Student gained valuable experience programming a practical application and will be featured as 2nd author on a pending publication.

Matthew Mollica, geology ('23). Created input data for simulations that tested the effect of different crop rotations on groundwater nitrate concentrations in a study well. Ran the model for

each set of scenarios and created appropriate figures to communicate the results. The student will be featured as 3rd author on a pending publication.

Community and Broader Impacts

The executable program developed through this project can be used by communities in Wisconsin, Minnesota, Michigan, and other regions whose municipal water supplies are derived from unconfined glacial aquifers to evaluate how changes in land use or water management influence the effective nitrate concentration in municipal water supplies. This is useful as a forensic tool to help identify the source of high nitrates within a well capture zone but also as a planning tool to prevent or mitigate nitrate pollution in municipal wells.

I have shared the model with the city of Waupaca in Waupaca, WI, and have taught the county GIS specialist how to generate new input data so that the county can use the model to develop and test their own scenarios that will inform local land and water-use decisions.

Scholarly Products

Pending Publications (Refereed Journal):

- DeVries, S., *Hooten, W.G., *Mollica, M. “A model for estimating nitrate in high-capacity wells as function of land use and time-of-travel capture zones in well-oxygenated sand and gravel aquifers.” – Pending submission to Environmental Software & Modeling (Impact Factor 4.807).

Refereed Technical Report:

- DeVries, S., Bradbury, K., and Cardiff, M. (2022). “A Groundwater Flow Model for Waupaca, WI.” Wisconsin Geological Survey and Natural History Survey Technical Report. 007, 88 p., https://doi.org/10.54915/xdis1726.

External Conferences:

- **Presentation:** “A modeling tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer.” Geological Society of America NC/SE Joint Sectional Meeting, Cincinnati, OH, April 7–8, 2022.
- **Poster:** “A modeling tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer.” Geological Society of America 2020 Connects Online Meeting, October 27, 2020.
- **Poster:** DeVries, S.L., *Hooten, W. (2020). A C++ tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer.” Fall Meeting of the American Geophysical Union.

Invited Talks:

- "A C++based model for estimating the concentration of nitrate at a municipal well in central Wisconsin." Presented to the Wisconsin Nitrate Task Force on August 21, 2020.

Presentations at UTC:

- **Poster:** DeVries, S.L., *Hooten, W. (2021). A C++ tool to estimate land-use impacts on groundwater nitrate concentrations observed at high-capacity pumping wells in an unconfined glacial aquifer." UTC Scholar ReSEARCH Dialogues.

Software:

Nitrate Calculator – A C++ executable program that estimates the annual average nitrate concentration of groundwater in a high-capacity pumping well using a look-up table of nitrate loss from USDA land cover classifications and gridded input data: time-of-travel capture zone, annual recharge depth, land cover.

The software is downloadable at:
https://github.com/garretthooten/NitrateCalculatorGUI/releases/tag/v1.2.1

Inventions or Other Intellectual Property

The executable file developed for this project is intended to be an open-access resource with potential use among water resource professionals.

Research Outreach & Collaboration

The executable file developed for this project is of immediate interest for several research collaborators and water resource professionals. It is expected to result in continued collaborations with:

- Bruce Rheineck, Program Manager, Drinking Water and Groundwater, Wisconsin DNR
- Brian Austin, Water Supply Specialist, Drinking Water and Groundwater, Wisconsin DNR
- Kenneth Bradbury, Director, Wisconsin Geologic and Natural History Survey
- Paul Juckem, Hydrologist, United States Geological Survey
- Michael Cardiff, Associate Professor, University of Wisconsin–Madison

Future collaboration with the above-listed individuals is anticipated to include further development of this tool so that it can be incorporated into a broader application called a nitrate decision support tool that will help relevant stakeholders (farmers, residents, state and local agencies, etc.) make land use and water management decisions that reduce the export of nitrate into groundwater resources.

EXTERNAL FUNDING

Proposal Submissions

No proposals related to this CEACSE award have yet been submitted.

Contracts/Awards Received

None to report.

Sponsored Program Capacity Building Activities

None to report.

WHAT'S NEXT FOR THIS RESEARCH?

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

I plan to continue working on the nitrate modelling program developed for this project. For example, the nitrate modelling program in its present form requires users to prepare ASCII files from land use raster datasets and from shapefiles that delineate the time required for water to travel from the land surface before it reaches a pumping well at depth. The former is a relatively simple procedure, but the latter is a relatively involved process that begins by importing polyline files from a groundwater flow model. This can be a time-limiting step, particularly if users wish to import capture zones that reflect different water management strategies. The next step in developing this tool will be to design and write a script in ArcGIS that will automatically generate capture zones and subdivide them into travel time by year for export as a raster dataset that can be read into the nitrate modeling program. This phase of the project can be completed in approximately 1 year. The next step would be to consult with collaborators working on a nitrate decision support tool to determine how to best incorporate the nitrate modeling program into existing frameworks developed to guide land nitrogen management.

Modifying the present nitrate model to account for different types of aquifer materials would be the next step. The present model is specific to surficial aquifers composed of unconsolidated glacial deposits and assumes that nitrate is conservative, i.e., it does not undergo any chemical transformations during transport and storage within the aquifer. The validity of this assumption is limited to the Great Lakes region of the United States. The model can be refined to include biodegradation equations that account for denitrification reactions that are typical of more carbon-rich and oxygen-depleted aquifers.

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

The support I received from CEACSE allowed me to set up a high-functioning workstation and remote modeling tools. Going forward, this situates me in pursuing additional modeling-based research questions, including the originally proposed question of whether a Thiessen-Polygon based subsurface model is statistically comparable to more complex geologic framework models. I see continued opportunities to work with government agencies, including the Wisconsin Department of Natural Resources and (hopefully) the Tennessee Department of Environment and Conservation to develop groundwater flow models and related resources that contribute to desired water quality and water supply outcomes.

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 greatest barrier to these next goals is time and finding students who have the computational background to contribute meaningfully to the project.

FINANCIAL ACCOUNTING

There are no remaining funds.

Fiscal Year 2022 Final Project Report

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

Eleni Panagiotou, Lead PI

Co-PI(s): Jin Wang, Abi Arabshahi, W. Y. Yang, Chris Dowell
Other Personnel: Evan Gildernew, Jarod Wright, Philip Smith, Dahlen Elstran

Project Title: A study on the local and global effects of polymer entanglement in material properties and biological functions

Date Submitted: 02/27/2017

Award Start–End Date: July 1, 2019–June 30, 2020

Non-Technical Summary:

This proposed research is focused on making the connection between microscopic and macroscopic properties in polymers and biopolymers. Our Objectives were to (1) link viscoelastic properties with polymer entanglement, (2) use the partitioned model simulation of polymers in order to account for fluid-structure interactions, and (3) conduct an experimental study of RNA to understand the relation between topology and biological function. Our outcomes showed (1) a direct relation between the periodic linking number and the molecular weight of polymers, while the viscoelastic response varied from the Rouse to the entangled regime, (2) the flattening of polymer knots/links in Couette flow, depending on the knot/link type, (3) the geometry of binders to RNA repeats related to disease share a similar pattern compared to non-binders. This research (1) contributes to the field of chemical engineering, polymer physics and mathematics by providing rigorous relations between polymer characteristics and their topology, (2) contributes to the field of chemical engineering, polymer physics and mathematics by providing rigorous relations between fluid flow of polymeric solvents and their topology, and (3) contributes to the field of biology and mathematics by providing a novel approach to detect binders to specific RNA sequences. During this time, three papers and eight presentations were published by E. Panagiotou. E. Gildernew was supported by the grant and presented his results in a poster at the UTC Research Dialogues, while the PI also mentored one undergraduate student in mathematics who was supported by the grant. J. Wang gave one talk. Y. W. Yong gave one presentation at a conference and mentored two undergraduate students supported by the grant. A. Arabshahi contributed research advice and expertise to the broader SimCenter infrastructure and C. Dowell contributed technical support in installing LAMMPS at the SimCenter computers and the cluster. E. Panagiotou and Jin Wang were awarded an NSF grant ($125,000). E. Panagiotou was awarded an NSF CAREER award. This project advanced or supported the mission of the SimCenter by obtaining external funding by publishing in peer-reviewed scientific journals and conferences where the SimCenter is mentioned and by training students.

PROJECT TITLE: A study on the local and global effects of polymer entanglement in material properties and biological functions

Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
• MD Simulation of polymer melts • Fluid-structure interaction simulations • Experiments on binding molecules to RNA sequences	Our results showed that the Periodic Linking Number of chains in a melt increase with their molecular weight and that there is a molecular weight beyond, which the viscoelastic response transitions from Rouse to entangled. The results were published in UTC Research Dialogues. Results related to this research about the role of polymer architecture, the effects of topology on proteins, and new topological measures were published by the PI in: Panagiotou E. and Kauffman L. H., 2020, Knot polynomials of open and closed curves *Proc. R. Soc. A* (accepted) Panagiotou, E. and Plaxco, K. W., 2020, A topological study of protein folding kinetics *Topology of Biopolymers, AMS Contemporary Mathematics Series* **746** Panagiotou E., Delaney K. T. and Fredrickson G. H., 2019, Theoretical prediction of an isotropic to nematic phase transition in bottlebrush homopolymer melts, *J. Chem. Phys.* **151**, 094901 and in 8 conferences and seminars. Our work on FSI fostered a new collaboration with ORNL (John Gounley). Our results show that a Couette flow flattens knots and links (our work is ongoing). E. Panagiotou and J. Wang applied and were awarded NSF support to continue working on this research. Our work on binders to RNA sequences shows some possible shared features of binders versus non-binders (this work is ongoing). This work was extended to find binders to the SARS-CoV-2 spike protein. Also, preliminary results show that the entanglement length in polymer melts coincide with a significant drop in the coefficient of the power of t^0 in the Jones polynomial.

RESULTS	OTHER INFO
N/A	**Budget and Schedule** Total Budget: $99,941.00 Actual Used: $99,941.00 Balance: $ 0 .00 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 • Publications (papers and presentations) • External and internal conference presentations **Organization Information** SimCenter, University of Tennessee at Chattanooga, eleni-panagiotou@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

This proposed research is focused on making the connection between microscopic and macroscopic properties in polymers and biopolymers. Understanding the effect of entanglement on the viscoelastic properties of material could lead to advanced manufacturing of material with desired properties. Similarly, understanding the effect of entanglement to the function of biopolymers could contribute to significant biological and medical applications such as site-specific drug delivery. The first part of this research focuses on studying the effects of entanglement and of fluid-structure interactions on the viscoelastic properties of polymeric material. The second part focuses on the effects of local and global geometrical and topological characteristics of RNA in search for site-specific binding molecules. Each one of the two research projects has three components:

1. The Molecular Dynamics (MD) simulation of polymers and biopolymers and their topological analysis.
2. The partitioned model simulation of polymers and biopolymers in order to account for fluid-structure interactions.
3. The experimental study of RNA polymeric systems in order to study their relation to polymer mechanics and function.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
MD simulations of varying molecular weight polymer melts in an oscillatory shear experiment	Completion of initial simulations, results presented in UTC Research Dialogues
Topological analysis of MD simulation results	Preliminary results obtained, working on the completion and on a manuscript. The results show that the entanglement length can be predicted from equilibrium conditions from the Jones polynomial of linear chains.
FSI simulations	Completion of simulation settings that can handle the FSI simulation of polymers, the study was extended to slip-link models of polymers
RNA repeats and binder analysis	Preliminary results suggest further analysis is needed. The results were extended to examine binders to the SARS-CoV-2 spike protein.
MD simulations of RNA repeats	Was not accomplished
New measures of topological entanglement	Creation of the Jones polynomial of open chains and creation of computational code in python

Challenges & Strategies Used to Address / Overcome:

We were not able to begin the MD simulations of RNA. The reason for this was the preliminary results on RNA and binder topological analysis took longer than expected, because it was difficult to obtain the experimental binder and non-binder molecules. In order to overcome this problem, one more graduate student would be required to work on the project with a focus on Molecular Simulation. The PI taught a course on Applied Knot Theory in fall 2020 to attract more students. A course on Molecular Simulation would have been helpful to attract qualified students.

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

The MD simulations of RNA repeats were not completed. A reason for this was that the training for the graduate students took longer than expected. I trained a student from the Department of Mathematics for four months but realized that he was not a good fit for the research, despite this effort. For this reason, I took an alternative approach, which used the optimized structures of binders to RNA instead of MD obtained structures. (This proved to be a beneficial idea in other contexts, which I am already working on and led to a part of a project related to COVID-19). The results on binder molecules to RNA so far are inconclusive but not negative. A reason for this is that we need more data. The data was obtained by co-PI, Y. W. Yong, by using an online software for obtaining optimized 3-D structures of binder molecules. This process was much slower than expected. There are two reasons for this: 1. not having free access to the gaussian program and 2. not having a student to work on this. From this I learned that it would be important to obtain a free access to the Gaussian program and train students in chemistry for using such chemical computational packages.

IMPACT & OUTCOMES

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

The PI had the chance to advise one graduate student in chemical engineering and one undergraduate student in mathematics. Also, she conducted research and published her work in peer-reviewed journals and in conferences and seminars. The PI and co-PI, Jin Wang, submitted and were awarded an NSF grant to work on this topic. The PI applied and was awarded an NSF CAREER award. The PI and co-PI, Jin Wang, established a new collaboration with ORNL in the framework of this grant.

The graduate student working with the PI, Evan Gildernew, had the chance to learn about Molecular Simulation and enhance his computational skills while also learning about Polymer Physics. He presented his results at UTC Research Dialogues and is continuing his work on this grant by writing a paper that will be submitted for publication at a peer-reviewed scientific journal.

The undergraduate student working with the PI, Peter Zeglen, had the chance to learn about applied knot theory and to enhance his computational skills. He graduated and is now working in the industry.

The co-PI, Y. W Yong, had the chance to advise two undergraduate students.

Students Impacted

Evan Gildernew, graduate student, MS in chemical engineering, participated in research and gave a poster presentation.

Peter Zeglen, graduated with a bachelor's in mathematics, participated in research.

Tanner Smith, PhD student in mathematics, initial training in research, (not funded by the grant due to insufficient interest and commitment).

Matthew Phanner, bachelor's in chemistry, participating in research.

Justin Pease, bachelor's in chemistry, participating in research

Community and Broader Impacts

The better understanding of entanglement in polymers can lead to manufacturing improved material with important industrial and biomedical applications and lead to the prevention of fatal diseases. The project was an interdisciplinary effort to bring together researchers from mathematics, chemistry, and the SimCenter. In addition, this grant trained students that learned and contributed to the projects.

The PI/co-PIs gave presentations to students, non-specialists, and multidisciplinary audiences and published in high impact peer reviewed mathematics and science journals.

Scholarly Products

Publications: All publications were in peer-reviewed scientific journals

- Panagiotou E. and Kauffman L. H., 2020, Knot polynomials of open and closed curves *Proc. R. Soc. A* (accepted)
- Panagiotou, E. and Plaxco, K. W., 2020, A topological study of protein folding kinetics *Topology of Biopolymers, AMS Contemporary Mathematics Series* **746**
- Panagiotou E., Delaney K. T. and Fredrickson G. H., 2019, Theoretical prediction of an isotropic to nematic phase transition in bottlebrush homopolymer melts, *J. Chem. Phys.* **151**, 094901

External Conferences:

- International Symposium, Polymers and networks, Ochanomizu University, Tokyo, Japan, August 2019.
- AMS Sectional Meeting University of California Riverside, November 2019
- Joint Mathematics Meetings, Denver, January 2020
- Topology Seminar, George Washington University, March 2020
- Program on Biological Physics of Chromosomes, KITP, June-July 2020 (virtual)
- Conference on Physical Knotting, Vortices and Surgery in Nature, Novosibirst State University, Russia, July 08, 2020 (virtual)
- Quantum Entanglement Seminar, Organized by L. H. Kauffman, July 09, 2020 (virtual)

- Women in Mathematics of Materials, Association of Women in Mathematics, SIAM, July 2020 (virtual)

The PI was planned to present the results in the following meetings, which were canceled due to COVID-19:

- AMS Sectional Meeting, University of Virginia
- Topology Workshop, Institute of Advance Study, April 2020, UPenn
- SIAM Conference on Mathematical Aspects of Materials Science, May 2020, Bilbao, Spain
- J. Wang, "Immersed boundary and immersed domain methods for fluid-structure interaction", Special Session on Applicable Analysis and Control Theory for Fluid and Fluid-Structure PDEs, SIAM
  Conference on Analysis of Partial Differential Equations, La Quinta, CA, December 2019.
- Y. W. Wang, talk at SERMACS 2019, October 2019

Presentations at UTC:

- Gildernew, Evan and Panagiotou, E. The effects of topological entanglement on viscoelastic properties of polymers, poster presentation at UTC Research Dialogues

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

The collaborator, Kumar Rajeev, Oak Ridge National Laboratories (ORNL), visited for 3 days (November 6–8, 2019) at the PI's institution, University of Tennessee at Chattanooga (UTC), and gave two seminars, one for the Department of Mathematics, UTC, and an interdisciplinary seminar for the SimCenter, UTC. During his visit, he worked with the PI on the creation of new methods to account for topological entanglement in Self Consistent Field Theory (SCFT). This work will provide methods to account for chain geometry/topology in this powerful theory for simulating polymers in large timescales.

A new collaboration was created with the PI, Jin Wang, and John Gounley from ORNL. The framework for FSI simulations has been created and tested for certain topologies.

EXTERNAL FUNDING

Proposal Submissions

- NSF Proposal on Entanglement in Polymers submitted prior to reporting period but immediately related to the proposed work.
- NSF CAREER: Topology of the active polymers (awarded)
- NSF MODULUS (not funded)
- ORAU Powe award (not funded)

Contracts/Awards Received

- NSF Proposal on Entanglement in Polymers, DMS Computational Mathematics, $125,000.
- NSF CAREER award: DMR and DMS, $537,000

Sponsored Program Capacity Building Activities

- Visited NSF to serve as reviewer. During that visit, I had planned meetings with two program officers in DMS Computational Mathematics and DMS Mathematical Biology
- Attended an NSF meeting at JMM meeting in Denver
- Attended workshops held for ORSP for preparing NSF CAREER proposals
- Organized BIRS meeting, 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 next year the PI will continue working on the entanglement of polymer melts and solutions. The PI and co-PI, Jin Wang, will continue working on the FSI simulations of entangled polymers. These results will shed light in the very complex relation between entanglement and fluid flow. Our results will lead to papers and possibly to new applications for external funding. The PI will continue working on using topology to finding binders to the spike protein of COVID-19.

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

I will pursue further collaboration with ORNL related to COVID-19. I will pursue research on active matter: entangled polymers with transient crosslinks. I will also pursue creating new measures of topological complexity with L. Kauffman, using Vassiliev invariants.

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?

An important barrier is the lack of interested graduate students. I have had difficulties finding students that can contribute to the mathematical research and I would like to support students from mathematics.

FINANCIAL ACCOUNTING

N/A