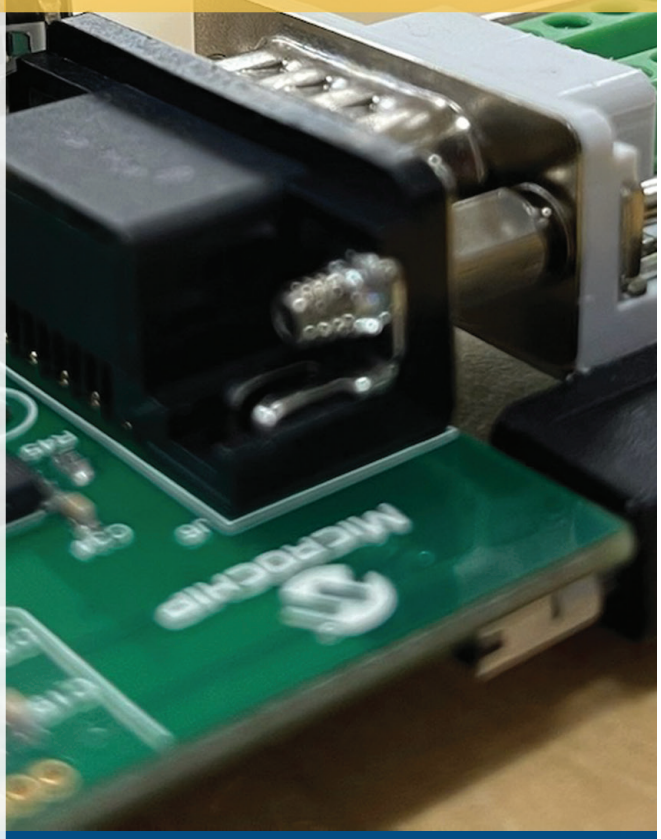
THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING



Annual Report to the Tennessee Higher Education Commission Fiscal Year 2020-2021

OCTOBER 15, 2021

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 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) continues its second decade of invigorating scientific inquiry, bolstering the learning environment, broadening participation, and establishing sustainable research pathways that benefit our institution, faculty and students, and the State of Tennessee. With our previous report for FY2020, CEACSE marked its 15th 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 FY2021 follows up our previous report with CEACSE's focused priority areas, highlights the ongoing strengths of its visionary leadership team, and notes greater impacts across a range of stakeholder groups. CEACSE comprises the indispensable factor that enables UTC to recruit, retain, and engage outstanding professors and equally outstanding students through research experiences for undergraduates up to and including PhD students.

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

Some notable outcomes in FY2021 include these highlights:

- From CEACSE funds, we awarded eight core awards ($100,000) and one Initiation/Opportunity Award ($15,000) in FY2021.
- We launched one new research thrust: Critical Infrastructure Protection (led by Dr. Don Reising).
- Dr. Andrew Bailey has developed new collaborations with Thrive Regional Partnership, The Trust for Public Land, Lula Lake, SORBA Chattanooga, Southeastern Climbers Coalition, Land Trust for TN, TN River Gorge Trust, Southeastern Conservation Corps, and WaterWays.
- Dr. Eleni Panagiotou submitted an NSF CAREER proposal related to her CEACSE project. It has been awarded.
- Dr. Sungwoo Yang received a Ruth S. Holmberg grant for his work. He also submitted a proposal to the NSF Engineering Research Initiative program.
- Dr. Abi Arabshahi submitted proposals to IBM on COVID-19 pulmonary airflow modeling and to the UT Biomedical Research Initiation Collaborative Grant program. The latter was funded.

- Dr. Reetesh Ranjan submitted proposals to NASA ULI, the DEPSCoR Research Collaboration program, and the ORAU Ralph E. Power Junior Faculty Enhancement Awards program.
- Dr. Reetesh Ranjan and his students created AVF-LESLIE, a fully compressible multi-species reacting flow solver, and UTCFOAM, an in-house and extended version of OpenFOAM.

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 emerging as a nexus of research incubation, HPC and data science, and a key provider of faculty resources that complement and supplement ORSP's offerings and add to those of faculty home departments.

This document constitutes the Annual Report for Fiscal Year 2021 of CEACSE activities and efforts. On behalf of UTC, SimCenter, our community partners and stakeholders, and our CEACSE-funded scientists and students, we express our deep appreciation to THEC for this critically important support of the CEACSE.

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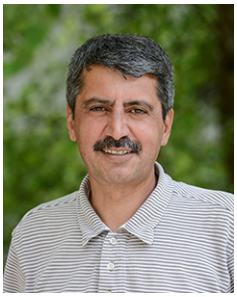
FACULTY & STAFF

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 FY2021 Awardees

The following faculty and staff were integral to the strategic direction of CEACSE during the 2020–2021 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. Abdollah Arabshahi



Abi Arabshahi is a SimCenter Research Professor. He received a BS (1982) in Civil Engineering and an MS (1985) and a PhD (1989) in Aerospace Engineering from Mississippi State University. His research interests include computational fluid dynamics, unsteady viscous flow applications, structured and unstructured grid technologies, autonomous underwater vehicles, internal and external aerodynamics and hydrodynamics, and computational bio-fluid dynamics. He has multiple publications in internationally reputable journals and conferences, as well as a book chapter, including *Frontiers of Computational Fluid Dynamics*, *AIAA Journal of Spacecraft and Rockets*, *International Journal of Computational Fluid Dynamics*, *Journal Physics Letters A, Journal of Nanomaterials, Scientific Reports Journal, Journal of Royal Society of Chemistry Advances, Applied Mathematics and Computation*, *International Journal of Systems*, *Journal of Franklin Institute*, *International Journal of Control*, and American Institute of Aeronautics and Astronautics (AIAA) and American Society of Mechanical Engineers (ASME) conferences.

Lead PI: "Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase Flows"

Dr. Andrew Bailey

Dr. Andrew Bailey teaches outdoor recreation, education and tourism in the Department of Health and Human Performance. He received his PhD in Education from the University of Minnesota, specializing in the use of outdoor activities and natural spaces to support human thriving. His research investigates the mutual benefits of the human/nature relationship, including economic impacts of outdoor recreation and tourism, as well as the psycho-physical benefits of exposure to natural environments.

Lead PI: "People, Planet and Profits: Strategic Planning for Outdoor Recreation, Conservation, and Tourism"

Dr. Michael Danquah

Dr. Danquah is a Professor of Chemical Engineering at the University of Tennessee at Chattanooga. His research focuses on the utilization of bioprocess and biomolecular engineering principles to develop emerging biopharmaceuticals; biosensing and molecular separation systems; environmental bioremediation systems; and biofuels and bio-products. His research findings are well published and cited with about 300 publications and a current H-index of 42. Dr. Danquah has served as a consultant to various companies including agricultural, pharmaceutical and biofuels industries. His work has resulted in several intellectual properties and commercial-scale manufacturing systems. He is a Chartered Engineer (CEng), a Chartered Scientist (CSci), a Fellow of the Institution of Chemical Engineers (FIChemE), and a Fellow of the Royal Society of Chemistry (FRSC). He was recently ranked in the top 2% of world scientists based on citations by a Stanford University publication.

Lead PI: "Real- SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics" [COVID-19 research]

Dr. Vahid Disfani

Dr. Vahid Disfani has been an Assistant Professor in the Department of Electrical Engineering at the University of Tennessee at Chattanooga since august 2017. He received his Bachelor degree from Amirkabir University of Technology, Iran in 2006, his M.S. degree from Sharif University of Technology, Iran in 2008, and his Ph.D. degree from the University of South Florida in 2015, all in Electrical Engineering. He continued his research as a postdoctoral scholar in the Center of Energy Research at the University of California San Diego in 2015-2017. His research fields of interest include Power system optimization and control, Grid integration of renewable energy resources, Distribution system optimal voltage regulation, Power markets and power system economics. His current research projects include comprehensive feeder-wide optimal voltage control, effective grid integration and optimal market participation of distributed energy resources, distributed and multi-agent optimal power flow for microgrids with high penetrations of renewable energy, reliability assessment of microgrids, and distributed algorithms for distribution systems state estimation.

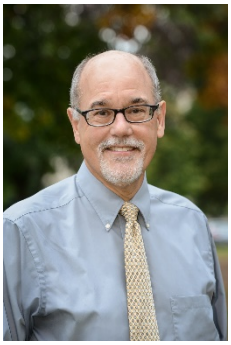
Lead PI: "Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources"

Dr. Loren Hayes

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. Gregory Heath



Gregory (Greg) W. Heath is Guerry Professor Emeritus in Public Health at the University of Tennessee at Chattanooga and Adjunct Professor of Medicine at the University of Tennessee Health Science Center College of Medicine Chattanooga. Prior to coming to Chattanooga, Dr. Heath spent over 20 years as an epidemiologist/health scientist with the U.S. Centers for Disease Control and Prevention (CDC). His undergraduate degree in psychology is from Westmont College (Santa Barbara, CA). Greg's graduate degrees are in epidemiology and nutrition/physiology from Loma Linda University School of Public Health in California. As an NIH trainee, he completed his postdoctoral fellowship in applied physiology at Washington University School of Medicine's Department of Preventive and Public Health (St. Louis, MO). Dr. Heath has spent his career devoted to the epidemiology, prevention, and management of chronic diseases and their associated behavioral risk factors (e.g., physical inactivity, poor diet, obesity) with a focus on health disparities among diverse populations (e.g., Native Americans, African Americans, Latinx/Hispanic Americans, and people with disabilities). His research has been funded through the NIH, CDC, American College of Sports Medicine, American Heart Association, and the Marshfield Clinic Medical Foundation. He is widely published in the preventive medicine and public health literature with 4 edited books and over 150 peer reviewed publications, book chapters, and scientific abstracts. Dr. Heath is a fellow in the American College of Sports Medicine (ACSM) and the American Heart Association's Council on Epidemiology and Prevention, and a member of the John Snow Society (Royal Society of Public Health, UK). *Co-Investigator*: "People, Planet and Profits: Strategic Planning for Outdoor Recreation, Conservation, and Tourism"

Dr. Soubantika Palchodhury

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

Lead PI: "Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19"

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 Topological Analysis of Viral Glycoproteins- Application to the Spike Protein of SARS-CoV-2" [COVID-19 funding]

"Topological design of porous metals for biomedical applications"

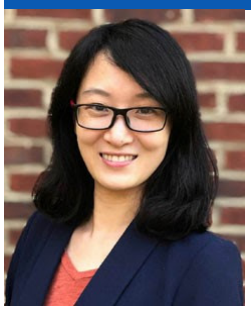
Dr. Reetesh Ranjan

Reetesh Ranjan is an Assistant Professor in the Department of Mechanical Engineering at the University of Tennessee at Chattanooga. He received MS and PhD in Theoretical and Applied Mechanics in 2009 and 2012, respectively, from the University of Illinois at Urbana-Champaign, and B. Tech. in Mechanical Engineering from the Indian Institute of Technology Kanpur in 2004. He worked at Ansys India from 2004 to 2007 as a Lead Application Engineer. He worked in the School of Aerospace Engineering at Georgia Tech from 2013 to 2019 as a postdoc, Research Engineer, and Senior Research Engineer. He conducts research in Fluid Mechanics and Thermal Sciences with a focus on the development of multi-fidelity computational methods and physics-based models for numerical investigation of multi-physics turbulent flows. These computational tools are used for a fundamental understanding of turbulence physics and its interaction with other processes in canonical configurations, predictive capabilities for flow and associated processes in practical configurations, and simulation-driven design. Some of the current applications of interests include turbulent flows in naval, rotorcraft, environmental and biomedical systems, reacting turbulent flows in energy conversion and propulsion devices, and energetic materials.

Co-Investigator: “Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase Flows”

*Lead PI: “*An Efficient Framework for Numerical Investigation of Turbulent Combustion Using Detailed Finite-Rate Chemistry”

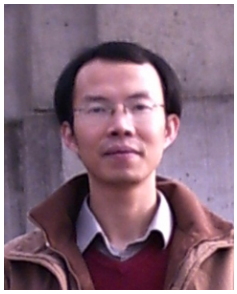
Dr. Yunye Shi



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. Jin Wang



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. Sungwoo Yang

Sungwoo Yang, an assistant professor, joined the Civil and Chemical Engineering Department at the University of Tennessee at Chattanooga (UTC) in the Fall of 2017. He received his PhD (2011) at Duke University, then joined MIT as a postdoctoral fellow to conduct research within the Device Research Laboratory (with Prof. Evelyn Wang). Later, he became a research scientist at MIT in 2014. The focus of his research is on porous materials which intersect the multidisciplinary fields of solar energy harvesting and water harvesting. He aims to bring about transformational efficiency enhancements in energy conversion and storage, buildings, water, and transportation by manipulating optical, thermal, and adsorptive properties of porous materials with device level considerations. The focus of his research efforts will be directed towards both: (1) fundamental research on developing new class of hybrid materials for efficient energy conversions and storages, and (2) applied research on devices and systems including for full spectrum solar energy conversion, thermal energy storage, water harvesting, and energy efficient buildings.

Lead PI: “A Low-Cost, Passive Solar Process Heat System”

FY2021 STUDENTS

Project Title: Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase Flows

Lead PI: Dr. Abdollah (Abi) Arabshahi

Students Impacted:

Timothy Johnston: Timothy Johnston is in the process of obtaining his master's degree in mechanical engineering. He plans to graduate in the fall semester with his thesis on particle-laden separating/reattaching flows. He was supported with a Graduate Research Assistantship for the Spring Semester of 2020 and has been receiving funding as a temporary research assistant otherwise.

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

Lead PI: Yunye Shi

Students Impacted:

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

Hannah Morgan: Hannah was introduced to the project and conducted basic analysis. Hannah is also pursuing for a master degree at UTC.

Project Title: Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources

Lead PI: Vahid Disfani

Students Impacted:

Pablo Macedo: Pablo was a master’s student and research assistant in Dr. Disfani’s research lab in the Electrical Engineering Department. He led Task 1 and 3 of the project. Throughout this project, he learned data processing, data visualization techniques, development of optimization models, and solving them using optimization solvers in MATLAB. Pablo wrote his and defended his M.S. thesis around the topic of this grant. He joined the power system industry in Fall 2021. He authored 2 conference papers from his involvement in this project.

Shailesh Wasti: Shailesh was a master’s student and research assistant in Dr. Disfani’s research lab in the Electrical Engineering Department. He led Task 2 of the project. Throughout this project, he learned data processing, data visualization techniques, development of optimization models, and solving them using optimization solvers in MATLAB. Shailesh co-authored 2 conference papers from his involvement in this project. Shailesh joined the Pennsylvania State University (Penn State) as a PhD student in Fall 2021.

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

Lead PI: Sungwoo Yang

Students Impacted:

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

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

Project Title: A Topological Analysis of Viral Glycoproteins- Application to the Spike Protein of SARS-CoV-2

Lead PI: Eleni Panagiotou

Students Impacted:

Quenisha Baldwin: Quenisha, a biology undergraduate student from Tuskegee University, submitted for publication 2 papers as first author, gave 3 talks on this work, and visited the group of Carolina Arias at UCSB to do experimental mutations on the Spike protein of SARS-CoV-2 to test our theoretical predictions.

Akua Maame Korsah: Akua (UTC, MS Math) proved the asymptotic scaling of the second Vassiliev measure of uniform random walks in confined space.

Arielle Beard: Ariell (Biology, UTC) worked on a related project under URTOPS and presented results at UTC Research Dialogues.

Achok Alier: Achok (Chem. Eng., UTC) worked on a related project under URTOPS and presented results at UTC Research Dialogues.

Project Title: People, Planet and Profits: Strategic Planning for Outdoor Recreation, Conservation, and Tourism

Lead PI: Andrew W. Bailey

Students Impacted:

Sarah Kelehear: (M.S. candidate-Environmental Science, Summer 2021) Sarah was involved in survey development and deployment, land manager communication, visitation estimation, GIS data acquisition and preparation, and field-based data collection. She was also the point person in identifying the Safegraph dataset and filtering the data for preliminary analyses. Sarah acquired full-time employment and exited the project in January 2021.

Jeremy Page: (M.S. candidate- Athletic Training, Summer 2021) Jeremy helped with survey data collection and field-based data collection for visitation and documentation of environmental issues. He was a main contact for local land managers and did a lot of data management for the Safegraph visitation data once it was in spreadsheets.

Brandon Denney: (M.S. candidate- Public Health, Summer 2021) Brandon handled the data acquisition and preparation for health and economic impacts for the 16 county region.

Alayna Smith: (B.S. SORT mgmt, May 2021) Alayna aided with visitation estimates, and field-based data collection of environmental issues on regional trails. Alayna presented visitation data from this project at the Southeastern Environment and Recreation Research (SERR) conference in March 2021. She was awarded the 3rd place overall prize for best undergraduate presentation.

Isaac Talbot: (B.S. SORT mgmt, May 2021) Isaac also aided with park visitation and field-based data collection. COVID issues limited his availability for much of the project.

Outdoor Recreation class (HHP 3060): This online course has involved 66 students in field-based data collections using the GIS collector app for iPhone and Android. Students documented 3 environmental issues on local trails to help establish a baseline from which to measure change over the next decade. They also collected information at trailheads regarding visitation, recreation user types, and tourism (i.e., license plate info). This process was valuable for them as they were taught various methods of visitor estimation and were introduced to GIS software utilized by all recreation & conservation land managers.

Project Title: An Efficient Framework for Numerical Investigation of Turbulent Combustion Using Detailed Finite-Rate Chemistry

Lead PI: Reetesh Ranjan

Students Impacted:

Jamie Bowers: (MS with thesis option, Summer 2021) Ms. Bowers learned carrying out high-fidelity turbulent combustion simulation using HPC resources. Additionally, she learned the skills to analyze large-scale datasets generated from simulations using Python. A key focus was to analyze statistical, structural, and spectral aspects of flame turbulence interactions prevalent in premixed flames. She has been trained on usage of tools such as AVF-LESLIE solver, Tecplot, Paraview, Python, GitHub, Latex, Trac, and Cantera.

Jash Doshi: (MS with non-thesis option, Spring 2021) Mr. Doshi was trained to carry out high-fidelity turbulent combustion simulation using HPC resources. He finished an independent study project focused on examining extinction and reignition occurring within a canonical non-premixed flame. He has been trained on usage of tools such as AVF-LESLIE solver, Tecplot, Paraview, Python, Trac, and Cantera.

Eli Durant: (Undergraduate, expected graduation Fall 2021) Mr. Durant has learned several skills ranging from pre- to post-processing and running the simulations using HPC resources provided by SimCenter. He has learned tools such as Python, Cantera, UTCFOAM, Tecplot, Paraview, Pointwise, Trac, etc.

Project Title: SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics

Lead PI: Michael Danquah

Students Impacted:

Godfred Sabbih: The project supported PhD student Godfred during the summer.

Project Title: Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19

Lead PI: Soubantika Palchoudhury

Students Impacted:

Syed Mohammad Tareq: Ph.D. student, summer stipend and research experience, expected graduation: 2023

Dell Zimmerman: Chemical Eng. undergraduate student, research training, graduation: 2021

Gitapun Jur: Chemical Eng. undergraduate student, summer research, graduation: 2023

Project Title: Climate and Social Evolution: Using Machine Learning to Improve Dataset Quality and to Develop Predictive Models

Lead PI: 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: 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.

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

Lead PI: Osama Osman

Students Impacted:

Jewel Rana Palit: MS student

Jibril Babatunde: MS student

Faiza Khan: MS student

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.

FY2021 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 Deans and faculty underpin this program.

Dr. Skjellum has led the CEACSE efforts for four 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 FY2022 and beyond.

The FY2021 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).

Advanced Modeling and Simulation R&D is now growing rapidly and with great promise its research thrust now has the most self-identified faculty and student participants. This area has been well represented in new external research awards received by CEACSE-funded projects. We have also created a new thrust: Critical Infrastructure Protection. This thrust provides a means to explore protection of critical infrastructure as described by the Department of Homeland Security. Dr. Don Reising converted the Energy thrust to Critical Infrastructure Protection, with the goal of focusing on the security aspect of energy. We are currently seeking funding to develop a center around this work, which is engaging and will involve many faculty on UTC's campus.

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 & Simulation
- Critical Infrastructure Protection (formerly Energy)
- Cybersecurity & Cyber-physical Systems
- Digital Twins
- Extreme Systems
- Health & Biological Systems
- High-Performance Computing & 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 undergo rigorous, double-blind, external review. 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 FY2021 as well, and CEACSE awardees are significant producers of external research proposals.

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

Overview of FY2021 Projects

In FY2021, the core CEACSE competition awarded new seed funding to support the research activities of 14 faculty members for eight new projects from various disciplines across computational science and engineering. From a total of 24 proposals, these nine were selected for their potential to continue CEACSE efforts to broaden the scope of research through increased participation of additional faculty, graduate students, and undergraduate students. Faculty Initiation and Opportunity Awards included one faculty member on one new project. Additional funding for COVID-19 research was granted to four faculty members on three new projects.

The funded projects key to the CEACSE/SimCenter priority areas active in FY2021: Advanced Modeling & Simulation, Cybersecurity & Cyber-physical Systems, Digital Twins, Energy, Environment, Health & Biological Systems, and High-Performance Computing & 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.

Core Competition

Project Title: A Low-Cost, Passive Solar Process Heat System
Lead PI: Sungwoo Yang
Co-PI(s): N/A
This project was extended into FY2022, due to issues resulting from COVID-19.

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

Project Title: An Efficient Framework for Numerical Investigation of Turbulent Combustion using Detailed Finite-Rate Chemistry
Lead PI: Reetesh Ranjan
Co-PI(s): N/A

Summary: Combustion devices such as liquid-fueled propulsion and gas turbine systems operating under lean conditions are desirable due to their low emission characteristics. Accurate prediction of complex physical processes observed in these devices—such as ignition, extinction, pollutant emissions, combustion instability, etc.—over a wide range of operating conditions requires the use of detailed finite-rate chemistry. Although recent computational advancements have enabled the use of detailed finite-rate chemistry while performing large-eddy simulation

(LES) of such systems, the computational expense tends to be huge, thus requiring further strategies for efficient computation. The proposed research focuses on establishing a novel computationally efficient framework for the investigation of turbulent combustion using detailed finite-rate chemistry. The framework will combine the two well-established approaches, namely the dynamic adaptive chemistry (DAC) approach with the hybrid transported-tabulated chemistry (HTTC) approach. While the DAC technique focuses on reducing the computational cost of the chemistry source term, the HTCC strategy reduces the total number of the transport equations by using self-similar profiles for the minor species while transporting only the major species. The novel computational framework will be verified and validated through well-established test cases corresponding to both premixed and non-premixed combustion configurations.

Project Title: Topological design of porous metals for biomedical applications
Lead PI: Eleni Panagiotou
Co-PI(s): Hamdy Ibrahim
This project was postponed to FY2022, due to issues resulting from COVID-19.

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

Project Title: Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications
Lead PI: Osama Osman
Co-PI(s): Farah Kandah
This project was postponed to 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: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models
Lead PI: Loren Hayes
Co-PI(s): Craig Tanis

This project was extended into 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: Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources
Lead PI: Vahid Disfani
Co-PI(s): Raga Ahmed

Summary: Grid integration of high penetration of distributed energy resources is expected to cause serious frequency excursions in power systems. These resources have highly intermittent power output and are connected through zero-inertia power electronic converters, both of which have adverse impacts on power system frequency. The main idea to resolve these issues is to emulate additional inertia through the same converters, which is referred to as virtual inertia. In addition to the total virtual inertia available throughout the power system, its allocation has a significant impacts on the frequency behavior of the power systems. This proposed project will develop real-time optimal allocation of virtual inertia in response to real-time forecast for availability of distributed energy resources. Realistic models of virtual inertia by different technologies will be developed. The optimization platform will be finally tested via software and real-time digital simulation platforms.

Project Title: People, planet, and profits: Strategic planning for outdoor recreation, tourism and conservation
Lead PI: Andrew Bailey
Co-PI(s): Greg Heath, Charlie Mix
This project was extended into FY2022, due to issues resulting from COVID-19.

Summary: This project will develop a decision-making tool for long-term recreation, conservation, and tourism planning, utilizing machine learning on multi-level data. Data on recreational use patterns, economic impact, physical activity and public health, biodiversity and conservation, and urban development and climate modeling will be geospatially analyzed to establish areas of high value and high vulnerability. This information will assist regional planners and municipalities in the development of strategic approaches to address public health, protection of biodiversity, and sustainable economic development through recreational and tourism assets. The relationship between recreational assets (i.e., parks, trails, and greenways), tourism impacts, conservation of biodiversity, and physical and mental health has been firmly established in previous research. However, the combined influence of these elements is rarely considered in regional planning models, likely due to a lack of resources. Open source and localized data, and modern machine-learning and geospatial techniques, render it feasible to develop a decision-making tool that accounts for the long-term health of people, the planet, and profits in regional planning. Situated in an area of high recreational value, rare and vulnerable biodiversity, but poor mental and physical health, this research team has a unique opportunity to identify key factors influencing the triple-bottom-line in a geospatial context.

Project Title: Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase flows
Lead PI: Abi Arabshahi
Co-PI(s): Reetesh Ranjan

Summary: The proposed research focuses on further enhancements in the Eulerian-Lagrangian (EL) formulation for large-eddy simulation (LES) of turbulent dispersed multiphase flows. Such flows are observed in several engineering applications and natural systems, and are comprised of a carrier phase and a dispersed phase. We consider the point-particle-based approximation within the EL formulation, where the carrier phase is simulated using a Eulerian approach and the dispersed phase is tracked in a Lagrangian manner. While the EL formulation is well established, there are several challenges associated with the Lagrangian evolution of the dispersed phase, particularly in the context of LES. We will focus on two key challenges, which include subgrid turbulence dispersion modeling and accuracy and efficiency aspects of parcel-based Lagrangian tracking. We will extend and evaluate three different strategies for subgrid dispersion under the same numerical framework, which include localized multi-scale approach, fractal interpolation technique, and approximate deconvolution method. The accuracy and convergence aspects of the parcel-based approach will be assessed by using deterministic and stochastic parcel-number-density control algorithms. The enhanced EL framework will be verified and validated through well-established test cases and will be used to investigate spray combustion and drug delivery applications.

Initiation/Opportunity Awards

Project Title: Predicting biomass gasification output: A machine learning approach
Lead PI: Yunye Shi
Co-PI(s): N/A

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 develop 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.

COVID-19 Projects

Project Title: A Topological Analysis of Viral Glycoproteins- Application to the Spike Protein of SARS-CoV-2
Lead PI: Eleni Panagiotou
Co-PI(s): N/A
This project was extended into FY2022, due to issues resulting from COVID-19.

Summary: A part of the viral life cycle involves viral recognition/binding with the host cell and subsequent fusion/penetration of cell or endosomal membrane (Dimmock 2007, Levine 1992). This research is focused on disrupting the ability of the viral glycoprotein to recognize its receptor or the ability to rearrange its three-dimensional conformation, thereby disrupting the viral life cycle. We propose to use topology to screen for binder molecules to the Spike protein of SARS-Cov-2 and for specific locations of binding along the Spike protein that would disrupt its function. More precisely, we propose to use topology to (1) predict residues of high conformational activity from a 3D structure and (2) to combine chemistry, topology and geometry to quantify the binding affinity of small molecules to the receptor binding domain of glycoproteins.

Project Title: SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics
Lead PI: Michael Danquah
Co-PI(s): N/A

Summary: Covid-19 has recently been announced by WHO as a pandemic disease with pneumonia-like complications. It is caused by the novel coronavirus SARS-CoV-2 and has been spreading rapidly in various countries worldwide. Transmission of the virus to humans mostly occurs via respiratory droplets from symptomatic and asymptomatic patients, as well as artifacts contaminated with the virus. Currently, the techniques used for Covid-19 diagnosis include Reverse-T Polymerase Chain Reaction, Isothermal Nucleic Acid Amplification, and Blood-Based Serological Tests. Whilst these methods have somewhat been useful in supporting Covid-19 mitigation efforts, they are challenged by several factors including long turnaround times, lack of specificity, false negative/positive results, and exhaustive sample preparation steps, amongst others. There is an urgent need for more robust, fast, and precise methods for Covid-19 diagnosis.

The SARS-CoV-2 virus is constructed by the assemblage of 4 distinct structural proteins, namely S (Spike glycoprotein), E (Envelope protein), M (Membrane protein) and N (Nucleoprotein). The N protein plays a key role in protecting the viral genome and its replication, the viral host infection process, and alteration of the host's immune response, making it an important functional target for the development of Covid-19 therapeutics. This project investigated how unique nucleic acid molecules called aptamers can be engineered to bind to the RNA-binding domains (RBD) of the N protein. Such bioprobes will be useful for rapid detection of the virus with high precision as well as offer targeted delivery of therapeutics to fight the virus. In this project, we accomplished successful construction of the structural models of the N protein of the virus and investigated conditions that enable high-affinity binding of the N protein to the aptamer. This preliminary work

has so far generated two extramural proposal submissions (one NSF and one NIH), and two journal articles which are currently under review. The funding also supported 1 PhD student.

Project Title: Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19
Lead PI: Soubantika Palchoudhury
Co-PI(s): Abi Arabshahi

Summary: A new panic zone RNA virus, severe acute respiratory syndrome coronavirus (SARS-CoV-2), has triggered the global pandemic of COVID-19, a pneumonia-like respiratory infection that has caused nearly one million deaths worldwide and has devastated the global economy. One of our key defenses against this deadly viral spread is early detection through testing and isolation of positive cases. SARS-CoV-2 can show an incubation period of 24 days and the virus can spread through asymptomatic individuals. This makes testing a priority to combat this pathogen. A point-of-care diagnostic test for COVID-19 will be a breakthrough innovation for our society, particularly for rural areas without adequate healthcare facilities. Current diagnostics for SARS-CoV-2 rely on reverse transcription polymerase chain reaction, immunoassays, and computed tomography. In this project, we aimed to realize a new and cost-effective point-of-care assay of high specificity and sensitivity for SARS-CoV-2. We designed this point-of-care assay by synthesizing novel biohybrid gold nanoparticle detection kit coupled with computational fluid dynamics predictions for suitable analyte concentrations. This flexible lateral flow paper assay will be further engineered as a pH-paper like colorimetric detection platform for the pathogen with a capability of result transmission via cellphone.

FY2021 Budget

NEW CORE AWARDS FY2021				
Lead PI	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Sungwoo Yang	A Low-Cost, Passive Solar Process Heat System	Energy	$86,771	$36,167**
Reetesh Ranjan	An Efficient Framework for Numerical Investigation of Turbulent Combustion using Detailed Finite-Rate Chemistry	Advanced Modeling & Simulation	$76,099	$67,978
Eleni Panagiotou	Topological design of porous metals for biomedical applications	Health & Biological Systems	$99,941	$71,211**
Osama Osman	Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications	Smart Cities & Urban Dynamics	$99,998	$87,171**
Loren Hayes	Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models	Health & Biological Systems	$98,662	$67,528**
Vahid Disfani	Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources	Energy	$92,942	$92,942
Andrew Bailey	People, planet, and profits: Strategic planning for outdoor recreation, tourism and conservation	Environment	$76,577	$51,681**
Abi Arabshahi	Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase flows	Advanced Modeling & Simulation	$99,221	$98,665
NEW INITIATION/OPPORTUNITY AWARDS FY2021				
Lead PI	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Yunye Shi	Predicting biomass gasification output: A machine learning approach	Energy	$15,000	$13,101

NEW COVID-19 AWARDS FY2021				
Lead PI	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Eleni Panagiotou	A Topological Analysis of Viral Glycoproteins-Application to the Spike Protein of SARS-CoV-2	Health & Biosystems	$19,965	$14,621**
Michael Danquah	SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics	Health & Biological Systems	$20,000	$20,000
Soubantika Palchoudhury	Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19	Health & Biological Systems	$20,000	$20,000

** *Due to COVID-19, some or all of the remaining funds on projects marked with asterisks were approved as carryover into FY2022 to support student researchers.*

Schedule 7

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution: UT Chattanooga **Center:** Computational Science & Engineering

	FY 2020-21 Actual			FY 2021-22 Proposed			FY 2022-23 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries									
Faculty	$104,943	$194,894	**$299,837**	$187,727	$348,636	**$536,363**	$140,246	$260,457	**$400,703**
Other Professional	$1,680	$3,120	**$4,800**	$3,005	$5,581	**$8,586**	$2,245	$4,170	**$6,415**
Clerical/ Supporting	$5,392	$10,013	**$15,405**	$9,645	$17,912	**$27,557**	$7,206	$13,382	**$20,587**
Assistantships	$78,074	$144,994	**$223,068**	$139,662	$259,372	**$399,034**	$104,338	$193,770	**$298,108**
Total Salaries	**$190,088**	**$353,021**	**$543,110**	**$340,039**	**$631,501**	**$971,540**	**$254,035**	**$471,778**	**$725,813**
Longevity	$594	$1,103	**$1,696**	$1,062	$1,973	**$3,035**	$794	$1,474	**$2,267**
Fringe Benefits	$29,365	$54,535	**$83,899**	$52,529	$97,554	**$150,083**	$39,243	$72,880	**$112,123**
Total Personnel	**$220,047**	**$408,659**	**$628,706**	**$393,630**	**$731,027**	**$1,124,658**	**$294,071**	**$546,132**	**$840,203**
Non-Personnel									
Travel	$442	$821	**$1,264**	$791	$1,469	**$2,260**	$591	$1,098	**$1,689**
Software	$15,270	$28,359	**$43,630**	$27,316	$50,731	**$78,047**	$20,407	$37,900	**$58,307**
Other Supplies	$9,136	$16,967	**$26,103**	$16,343	$30,351	**$46,694**	$12,209	$22,674	**$34,884**
Equipment	$50,551	$93,881	**$144,432**	$90,428	$167,938	**$258,367**	$67,557	$125,463	**$193,019**
Scholarships	$6,375	$11,840	**$18,215**	$11,404	$21,180	**$32,584**	$8,520	$15,823	**$24,343**
Other (Specify):									
Print	$620	$1,151	**$1,771**	$1,109	$2,059	**$3,168**	$828	$1,538	**$2,367**
Other Personal Services	$10,483	$19,468	**$29,951**	$18,752	$34,825	**$53,577**	$14,009	$26,017	**$40,026**
Special Commercial Services	($8,084)	($15,014)	**($23,098)**	($14,462)	($26,857)	**($41,319)**	($10,804)	($20,064)	**($30,868)**
Memberships	$159	$295	**$454**	$284	$528	**$812**	$212	$394	**$607**
Student Fees	$27,055	$50,246	**$77,301**	$48,398	$89,882	**$138,280**	$36,157	$67,148	**$103,305**
Total Non-Personnel	**$112,008**	**$208,014**	**$320,022**	**$200,364**	**$372,105**	**$572,470**	**$149,687**	**$277,991**	**$427,678**
GRAND TOTAL	**$332,055**	**$616,673**	**$948,728**	**$593,995**	**$1,103,133**	**$1,697,127**	**$443,758**	**$824,123**	**$1,267,881**
Revenue									
New State Appropriation		$800,516	**$800,516**		$821,220	**$821,220**		$862,281	**$862,281**
Carryover State Appropriation		$151,507	**$151,507**		$335,350	**$335,350**		$0	**$0**
New Matching Funds	$405,600		**$405,600**	$405,600		**$405,600**	$405,600		**$405,600**
Carryover from Previous Matching Funds	$61,412		**$61,412**	$134,957		**$134,957**	$0		**$0**
Total Revenue	**$467,012**	**$952,023**	**$1,419,035**	**$540,557**	**$1,156,570**	**$1,697,127**	**$405,600**	**$862,281**	**$1,267,881**

Schedule 7

FY2021 PUBLICATIONS AND PRESENTATIONS (of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings

Assessment of Subgrid Dispersion Models for Large-Eddy Simulation of Particle-Laden Turbulent Flows, AIAA Scitech, 2021. **(Abdollah (Abi) Arabshahi**)

"Predicting Steam-Gasification Output Using Artificial Neural Networks" has been accepted for IMECE 2021 for both publication and conference presentations. **(Yunye Shi)**

Q. Baldwin, Applied Knot Theory Workshop 2020, UTC (**Eleni Panagiotou**)

Q. Baldwin, AMS Southeastern Fall Sectional meeting 2020, Contributed Session, UTC (**Eleni Panagiotou**)

E. Panagiotou, BMSE/MCDB joint seminar, UCSB

Q. Baldwin, Research Dialogues 2021, UTC, (**Eleni Panagiotou**)

Arielle Beard and Achok Alier, Research Dialogues 2021, UTC (**Eleni Panagiotou**)

Bailey, A. & Smith, A. (2021). Of parks and pandemics: Visitation disparities across county lines. Presentation for the Southeastern Recreation Research Conference (virtual, refereed); March, 2021

Bailey, A. & Smith, A. (2021). Of parks and pandemics: Visitation disparities across county lines. Presentation for UTC Research Dialogues (virtual); March, 2021

Bailey, A., Heath, G.W., & Mix, Charlie (2021). People, Planet, & Profits: Strategic planning for outdoor recreation, tourism, and conservation (virtual). A CEACSE presentation for UTC Research Dialogues; March, 2021

Application of Intrusive and Non-Intrusive Reduced Order Modeling Techniques for Simulation of Turbulent Premixed Flames, AIAA Propulsion and Energy Forum and Exposition, 2021 (Presenter: **R. Ranjan**).

Application of Hybrid Transported-Tabulated Chemistry for Efficient Large Eddy Simulation of Turbulent Premixed Combustion, AIAA SciTech Forum and Exposition, 2021 (Presenter: **R. Ranjan**).

Numerical Investigation of the Effects of Elevated Pressure and Chemistry on the Characteristics of Turbulent Premixed Flames, Research Dialogues, UTC, 2021 (Presenter: J Bowers). (**Reetesh Ranjan**)

Simulation of Extinction And Re-Ignition Events in a Turbulent Non-Premixed Flame, CECS Tech Symposium, UTC, 2021 (Presenter: J. Doshi). (**Reetesh Ranjan**)

Effect of Pressure on Heat Release and Curvature Statistics of Turbulent Premixed Flame, CECS Tech Symposium, UTC, 2021 (Presenter: J Bowers). (**Reetesh Ranjan**)

Large Eddy Simulation of the Volvo Bluff Body Flame Experiment, CECS Tech Symposium, UTC, 2021 (Presenter: E. Durant). (**Reetesh Ranjan**)

Suggs, E.D. 2019. Meta-textual analysis of biological research. ACM meeting, Gatlinburg, TN. (**Loren Hayes**)

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.

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

P. Ubiratan, S. Wasti, and **V. Disfani**, “Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm,” in 2020 IEEE International Conference on Smart Grid Communications (Smart-GridComm), IEEE, 2020.

P. Ubiratan, S.Wasti, and **V. Disfani**, “Frequency Deviation Controller for Inter-Area Oscillations Damping in Smart Grids,” in 2021 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT), IEEE, 2021.

P. Ubiratan, “Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021. (**Vahid Disfani**)

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

Oral talk at Materials Research Society Annual Conference, Virtual Meet, 2020. (**Sou Palchoudhury**)

Biophysical analysis of SARS-CoV-2 transmission and theranostic development via N protein computational characterization. Biotechnology Progress (Accepted for publication) (**Michael Danquah**)

Engineered Aptamers for Enhanced COVID-19 Theranostics. Cellular and Molecular Bioengineering (Under Review) (**Michael Danquah**)

Software

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

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

Refereed Publications

A paper entitled “Predicting Steam-Gasification Output via Machine Learning Approaches” is under review in Energy. (**Yunye Shi**)

Baldwin, Q. and **Panagiotou E.**, 2021, The local topological free energy of proteins Journal of Theoretical Biology (under minor revision)

Baldwin, Q., Sumpter, B. G. and **Panagiotou E.**, 2021, The local topological free energy of the SARS-CoV-2 spike protein (submitted-under revision)

Panagiotou, E., Vuong, V. Q., Irle, S. and Sumpter, B. G., 2021, Geometry as a screening tool for strong binders to the SARS-CoV-2 Spike protein (submitted)

J. Bowers, E. Durant, and **R. Ranjan**, “Application of Intrusive and Non-Intrusive Reduced Order Modeling Techniques for Simulation of Turbulent Premixed Flames”, AIAA-2021-3634.

V. Hasti and **R. Ranjan**, “Analysis of Flame Structure During Longitudinal Combustion Instability within a High-Pressure Shear Coaxial Single Element Combustor”, Accepted for Symposium on Thermoacoustics in Combustion: Industry meets Academia (SoTiC 2021), 2021.

J. Bowers, E. Durant, and **R. Ranjan**, “On the Effects of Variation of Pressure, and Length- and Velocity-Scale Ratios on the Features of Methane/Air Turbulent Premixed Flames”, Under Preparation, 2021.

A. Panchal, S. Karpe, **R. Ranjan**, and S. Menon, “Application of Hybrid Transported-Tabulated Chemistry for Efficient Large Eddy Simulation of Turbulent Premixed Combustion”, Under Preparation, 2021.

Olivier, C, Jaeggi, A., **Hayes, L.D.**, & Schradin, S. Revisiting Macroscelidea social systems: Evidence for variable social organization, including pair-living, but not for a monogamous mating system. Submitted to Journal of Mammalogy.

P. Ubiratan, S. Wasti, and **V. Disfani**, “Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm,” in 2020 IEEE International Conference on Smart Grid Communications (Smart-GridComm), IEEE, 2020.

P. Ubiratan, S.Wasti, and **V. Disfani**, “Frequency Deviation Controller for Inter-Area Oscillations Damping in Smart Grids,” in 2021 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT), IEEE, 2021.

P. Ubiratan, “Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021. (**Vahid Disfani**)

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

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

Patent Applications

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

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

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

EXTERNAL FUNDING

Abdollah (Abi) Arabshahi, Lead PI

Co-PI(s): Dr. Reetesh Ranjan
Other Personnel: Timothy Johnston – Graduate Student Researcher

Project Title: Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase Flows

Proposal Submissions

1. Research proposal entitled, "COVID-19-Patient-Specific HPC Simulation of Pulmonary Airflow Structure and Aerosol Particles Transport/Deposition Patterns," to the IBM Faculty Award Technical Discovery, PI, $50,000, target submission March 2021.
2. Research proposal white paper entitled, "High-Performance Numerical Simulation of Flow Structures and Transport/Deposition of Particles in Pulmonary Airways in Support of COVID-19 treatments in hospitalized and long-haul patients," submitted to the National Science Foundation's Leadership Class Computing Facility (NSF's LCCF), PI, $120,000 - $150,000 per year, February 26, 2021.
3. UT Biomedical Research Initiation Collaborative Grants, "Computational Investigation of Region Aerosol Deposition in Realistic Human Airways," Co-PI, $24,920, January 1, 2020 to December 31, 2020.
4. Department of Energy (DOE), "PSAAP-III (FIC): Center for Understandable, Performant Exascale Communication Systems (CUP-ECS)," Senior Personnel, $1.3M (UTC portion), July 1, 2020 to June 30, 2025.
5. National Science Foundation (NSF), "Collaborative Research: Software Engineering Workforce Development in High Performance Computing for Digital Twins," Co-PI, $57,635, October 1, 2019 to September 30, 2021.
6. National Science Foundation (NSF), "RUI: Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems," PI, $42,269, August 1, 2019 to July 31, 2021.
7. Research proposal white paper entitled, "A Data-Driven Multi-Parameter Reduced Order Modeling Framework for Investigation of Hypersonic Systems," PI, $887,427, AFOSR # FOA-AFRL-AFOSR-2020, 05/01/2021 - 04/30/2024.
8. Research proposal entitled,"COVID-19-Relevant Computational Modeling of Human Respiratory Airways," PI, $1,222,244, PRMPR-IIRA-2020, DOD- Department of the Army, USAMRAA,10/01/2021 - 9/30/2025.
9. Research proposal entitled, "STOP COVID: Stopping Transmission of Airborne Pathogens in Confined spaces Via Integrated Designs," Co-PI, $1,599,432, W81XWH-20-PRMPR-IIRA-COVID, DOD-Department of the Army, USAMRAA, 10/01/2021-9/30/2025.

Contracts/Awards Received

1. UT Biomedical Research Initiation Collaborative Grants, "Computational Investigation of Region Aerosol Deposition in Realistic Human Airways," Co-PI, $24,920, January 1, 2020 to December 31, 2020.
2. Department of Energy (DOE), "PSAAP-III (FIC): Center for Understandable, Performant Exascale Communication Systems (CUP-ECS)," Senior Personnel, $1.3M (UTC portion), July 1, 2020 to June 30, 2025.

3. National Science Foundation (NSF), “Collaborative Research: Software Engineering Workforce Development in High Performance Computing for Digital Twins,” Co-PI, $57,635, October 1, 2019 to September 30, 2021.
4. National Science Foundation (NSF), “RUI: Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems,” PI, $42,269, August 1, 2019 to July 31, 2021.

Yunye Shi, Lead PI

Co-PI(s): none
Other Personnel: none

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

Proposal Submissions

1. NSF ERI submitted in 2021 Summer
2. UTC CEACSE submitted in 2020 Fall

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. Several NSF grant webinars
2. College grant writing workshops

Vahid Disfani, Lead PI

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

Project Title: Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources

Proposal Submissions

1. One NSF CAREER Proposal in July 2020.

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. I attended NSF CAREER workshop set up by NSF in February 2021, after my first submission in 2020.

Sungwoo Yang, Lead PI

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

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

Proposal Submissions

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

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Eleni Panagiotou, Lead PI

Co-PI(s): N/A
Other Personnel: Quenisha Baldwin, Akua Maame Korsah

Project Title: A Topological Analysis of Viral Glycoproteins- Application to the Spike Protein of SARS-CoV-2

Proposal Submissions

NSF CAREER: Topology of active polymers (recommended for funding)

Contracts/Awards Received

NSF Proposal on Entanglement in Polymers, DMS Computational Mathematics, $125,000.

Sponsored Program Capacity Building Activities

Visited (virtually) NSF to serve as a reviewer.

Reetesh Ranjan, Lead PI

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

Project Title: An Efficient Framework for Numerical Investigation of Turbulent Combustion Using Detailed Finite-Rate Chemistry

Proposal Submissions

1. Numerical investigation of effects of condensed and gas-phase finite-rate kinetics on the flame structure and surface regression in solid propellant combustion, White Paper, Propulsion, and Energetics Program, DEPSCOR, 2020.
2. A low emission combustion system for high overall pressure ratio compact core engines, Stage A Proposal, NASA ULI, 2020.

3. Reduced-Order Modeling Techniques for Efficient Simulation of Turbulent Combustion, 2021 ORAU Ralph E. Powe Junior Faculty Enhancement Awards, 2021.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Michael Danquah, Lead PI

Other Personnel: Michael Danquah, Dr

Project Title: SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics

Proposal Submissions

1. Wireless electrochemical aptasensing of SARS-CoV-2 nucleoproteins for rapid Covid-19 diagnosis and telehealth applications. NIH R15. Lead PI
2. Collaborative Research: RUI: Spike protein and ACE2 binding checkpoint for rapid screening of SARS-CoV-2 from saliva via nanostructured bijeltemplated electrochemical biosensor. NSF RUI. Lead PI

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Dr. Soubantika Palchoudhury, Lead PI

Co-PI(s): Prof. Abdollah Arabshahi

Project Title: “Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19”

Proposal Submissions

1. Investigating the dynamics and therapeutics for SARS-CoV-2 through an integrated computational and experimental approach, American Lung Association, $200,000
2. Investigating the dynamics and therapeutics for SARS-CoV-2 through an integrated computational and experimental approach, National Institute of Allergy and Infectious Diseases, $137,500

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

1. Consultations with NSF IRES program officer.
2. Managed my NSF IRES grant.

OVERVIEW OF FY2022 PROJECTS

The following awardees and projects, selected for funding in February 2021, are currently supporting CEACSE's strategic goals and future plans for FY2022. 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: A Low-Cost, Passive Solar Process Heat System
Investigators: Sungwoo Yang
Thrust: Energy
Amount: $82,771

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

Title: An Efficient Framework for Numerical Investigation of Turbulent Combustion using Detailed Finite-Rate Chemistry
Investigators: Reteesh Ranjan
Thrust: Advanced Modeling & Simulation
Amount: $76,099

Abstract: Combustion devices such as liquid-fueled propulsion and gas turbine systems operating under lean conditions are desirable due to their low emission characteristics. Accurate prediction of complex physical processes observed in these devices—such as ignition, extinction, pollutant emissions, combustion instability, etc.—over a wide range of operating conditions requires the use of detailed finite-rate chemistry. Although recent computational advancements have enabled the use of detailed finite-rate chemistry while performing large-eddy simulation (LES) of such systems, the computational expense tends to be huge, thus requiring further strategies for efficient computation. The proposed research focuses on establishing a novel computationally efficient framework for the investigation of turbulent combustion using detailed finite-rate chemistry. The framework will combine the two well-established approaches, namely the dynamic adaptive chemistry (DAC) approach with the hybrid transported-tabulated chemistry (HTTC) approach. While the DAC technique focuses on reducing the computational cost of the chemistry source term, the HTCC strategy reduces the total number of the transport equations by using self-similar profiles for the minor species while transporting only the major species. The

novel computational framework will be verified and validated through well-established test cases corresponding to both premixed and non-premixed combustion configurations.

Title: Topological design of porous metals for biomedical applications
Investigators: Eleni Panagiotou, Hamdy Ibrahim
Thrust: Health & Biological Systems
Amount: $92,955

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

Title: Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications
Investigators: Osama Osman, Farah Kandah
Thrust: Smart Cities
Amount: $99,998

Abstract: 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.

Title: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models
Investigators: Loren Hayes, Craig Tanis
Thrust: Health & Biological Systems
Amount: $98,662

Abstract: 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.

Title: Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources
Investigators: Vahid Disfani, Raga Ahmed
Thrust: Energy & Environment
Amount: $92,942

Abstract: Grid integration of high penetration of distributed energy resources is expected to cause serious frequency excursions in power systems. These resources have highly intermittent power output and are connected through zero-inertia power electronic converters, both of which have adverse impacts on power system frequency. The main idea to resolve these issues is to emulate additional inertia through the same converters, which is referred to as virtual inertia. In addition to the total virtual inertia available throughout the power system, its allocation has a significant impacts on the frequency behavior of the power systems. This proposed project will develop real-time optimal allocation of virtual inertia in response to real-time forecast for availability of distributed energy resources. Realistic models of virtual inertia by different technologies will be developed. The optimization platform will be finally tested via software and real-time digital simulation platforms.

Title: People, planet, and profits: Strategic planning for outdoor recreation, tourism and conservation
Investigators: Andrew Bailey, Greg Heath, Charlie Mix
Thrust: Health & Biological Systems + Environment
Amount: $76,577

Abstract: This project will develop a decision-making tool for long-term recreation, conservation, and tourism planning, utilizing machine learning on multi-level data. Data on recreational use patterns, economic impact, physical activity and public health, biodiversity and conservation, and urban development and climate modeling will be geospatially analyzed to establish areas of high value and high vulnerability. This information will assist regional planners and municipalities in the development of strategic approaches to address public health, protection of biodiversity, and sustainable economic development through recreational and tourism assets. The relationship between recreational assets (i.e., parks, trails, and greenways), tourism impacts, conservation of biodiversity, and physical and mental health has been firmly established in previous research. However, the combined influence of these elements is rarely considered in regional planning models, likely due to a lack of resources. Open source and localized data, and modern machine-learning and geospatial techniques, render it feasible to develop a decision-making tool that

accounts for the long-term health of people, the planet, and profits in regional planning. Situated in an area of high recreational value, rare and vulnerable biodiversity, but poor mental and physical health, this research team has a unique opportunity to identify key factors influencing the triple-bottom-line in a geospatial context.

Title: Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase flows
Investigators: Abi Arabshahi, Reetesh Ranjan
Thrust: Advanced Modeling & Simulation + Health & Biological Systems
Amount: $92,991

Abstract: The proposed research focuses on further enhancements in the Eulerian-Lagrangian (EL) formulation for large-eddy simulation (LES) of turbulent dispersed multiphase flows. Such flows are observed in several engineering applications and natural systems, and are comprised of a carrier phase and a dispersed phase. We consider the point-particle-based approximation within the EL formulation, where the carrier phase is simulated using a Eulerian approach and the dispersed phase is tracked in a Lagrangian manner. While the EL formulation is well established, there are several challenges associated with the Lagrangian evolution of the dispersed phase, particularly in the context of LES. We will focus on two key challenges, which include subgrid turbulence dispersion modeling and accuracy and efficiency aspects of parcel-based Lagrangian tracking. We will extend and evaluate three different strategies for subgrid dispersion under the same numerical framework, which include localized multi-scale approach, fractal interpolation technique, and approximate deconvolution method. The accuracy and convergence aspects of the parcel-based approach will be assessed by using deterministic and stochastic parcel-number-density control algorithms. The enhanced EL framework will be verified and validated through well-established test cases and will be used to investigate spray combustion and drug delivery applications.

Faculty Initiation/Opportunity Award

Title: Predicting Biomass Gasification Output – A Machine Learning Approach
Investigator: Yunye Shi
Thrust: Energy
Amount: $15,000

Abstract: 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

CONCLUSION

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

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

CEACSE-supported initiatives have already formed the basis of several collaborations and partnerships with other institutions of higher education and with business and industry partners. A number of meaningful Memoranda of Understanding and Non-Disclosure Agreements have been executed between UTC and a variety of partners and potential sponsors to explore how CEACSE can support engineering enhancements, address regional and state priority areas, and bolster robust economic growth.

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 FY2021 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

Raga Ahmed, Ph.D.
Associate Professor
Electrical Engineering Department
College of Engineering and Computer Science
University of Tennessee at Chattanooga
Chattanooga, TN

a. Professional Preparation

University of Khartoum, Khartoum, Sudan, Electrical Engineering, BSc, 1988
Rice University, Houston, TX, Electrical Engineering, MEE, 2003
Georgia Institute of Technology, Atlanta, GA, Electrical Engineering, Ph.D, 2013

b. Appointments

2019-present	Associate Professor, Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, TN
2013-2019	Assistant Professor, Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, TN
2011-2012	Adjunct Instructor, Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, TN
2009-2011	Equity and Diversity Fellow (Instructor), Electrical Engineering Department, University of Tennessee at Chattanooga (UTC), Chattanooga, TN
2001-2004	Research Engineer, Moog/Litton-Polyscientific, Marietta, GA
1994-1997	System Analyst, Operation Simulation Associates, Ringgold, Georgia

c. Products

(i) 5 Selected Products (*Student Author)

1. *B. Cedano, A. Eltom, B. Hay, J. Glass, R. Ahmed, “A fully-automated Disturbance Analysis Vision for the Smart Grid Based on Smart Switch Data”. International Journal of Electrical, Computer, Energetic, Electronic and Communication Engineering, Vol. 12, no. 6, pp 487-494 July, 2018.

2. *N. A. Boakye-Boateng and R. Ahmed, "A Windows-Based Framework for Enhancing Scalability and Reproducibility of Large-scale Research Data," 2018 ASEE Southeastern Section Conference, Mar. 2018.

3. *Hana Karrar, Neslihan Alp, Louie Elliott, Raga Ahmed, Trevor Elliott, Li Yang, and Mbaki Onyango, “Girls to Engineeris Network”, 2018 International Conference of the American Society of Engineering Management.

4. *N. A. Boakye-Boateng and R. Ahmed, "Effects of Tooth Geometry on the Operating Characteristics of Linear Variable Reluctance Motors with Coupled Flux Paths," IEEE Southeastcon 2018. Apr. 2018

5. *N. A. Boakye-Boateng and R. Ahmed, "Characterization and modeling of a linear variable reluctance motor considering a full range of feasible tooth widths with finite element method," 2017 IEEE Industry Applications Society Annual Meeting, Cincinnati, OH, 2017, pp. 1-7.

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

1. *B. Cedano, A. Eltom, B. Hay, J. Glass, R. Ahmed, “A fully-automated Disturbance Analysis Vision for the Smart Grid Based on Smart Switch Data”. ICRERA, Paris, France, July 25-26, 2018.

2. *M. A. Saad, A. H. Eltom, G. L. Kobet, R. Ahmed. Performance Comparison between DualBlinder and Phasor-Based Out-of-Step Detection Functions Using Hardware-in-the Loop Simulation, IEEE Industrial Applications Society, Oct 2015.

3. R. Ahmed, D. Taylor, "Targeted-ripple optimal commutation of coupled and uncoupled linear variable reluctance motors," *IEEE Southeastcon 2015*, pp. 1-8, April 2015.

4. R. Ahmed and D. G. Taylor, "Assessment of linear variable reluctance motor performance limits via finite element modeling," *Proceedings of the International Conference on Electrical Machines,* Chania, Greece, 6 pages on CD-ROM, September 2006.

5. R. Ahmed and D. G. Taylor, "Optimal excitation of linear variable reluctance motors with coupled and uncoupled flux paths," *Proceedings of the IEEE International Symposium on Industrial Electronics*, Montreal, Canada, pp. 2498--2503, July 2006.

d. Synergistic Activities

1. Principal Investigator, NST "RET Site: Engineering and Data Analytics in Smart Cities", $595,536, September 1, 2019 – September 1, 2022.

2. Senior personnel, NSF Research Experience for Undergraduates (REU), "REU Site: An Interdisciplinary CubeSat Research and STEM Education Platform at the University of Tennessee at Chattanooga (UTChattSat)," $359,783, Mar. 2018-Feb. 2021.

3. Co-PI, Engineering Information Foundation, EIF, "UTC Girls to Engineers Network (GEN) Funding Priority - Programs to Encourage Middle School Girls in Engineering", $14,586, May 2017–August 2018.

4. Coach, First Lego League, Girls and their Robots team of Chattanooga Girls Leadership Academy, 2017-present

5. Faculty Advisor, UTC Student Chapter, National Society of Black Engineers (NSBE), 2016-present.

ABDOLLAH (ABI) ARABSHAHI
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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.”

Andrew W. Bailey, Ph.D.
UC Foundation Associate Professor, Health and Human Performance
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(a) *Professional Preparation*

Johnson University	Knoxville, TN	Theology/Education	B.S. 1998
University of Tennessee	Knoxville, TN	Rec. Parks. Tourism	M.S. 1999
University of Minnesota	Minneapolis, MN	Education	Ph.D. 2009

(b) *Appointments*

2012-present	UC Foundation Associate Professor, University of TN, Chattanooga; Chattanooga, TN. Department of Health and Human Performance; Teaching, research, curriculum development, community planning & engagement (Tenured 2017).
2009-2012	Assistant Professor, Calvin College; Grand Rapids, MI. Department of Kinesiology; Teaching, advising, research, course development.
2006-2009	Instructor & Graduate Assistant, University of Minnesota, Twin Cities, Department of Recreation Parks and Leisure Studies; Teaching, research, marketing and PR, course development.

(c) *Related Publications*

1) Bailey, A. W., & Hamilton, K. (2019). Engineering physical activity into daily life through public space. *ACSM's Health & Fitness Journal*, *23*(5), 45. https://doi.org/10.1249/FIT.0000000000000511
2) Bailey, A. W., & Hungenberg, E. (2018). Managing the rock-climbing economy: A case from Chattanooga. *Annals of Leisure Research*, *0*(0), 1–19. https://doi.org/10.1080/11745398.2018.1488146
3) Bailey, A., & Russell, K. C. (2010). Predictors of interpersonal growth in volunteer tourism: A latent curve approach. *Leisure Sciences*, *32*(4), 352–368.
4) Bailey, A., & Fernando, I. (2012). Routine and project-based leisure, happiness and meaning in life. *Journal of Leisure Research*, *44*(2), 139–154.
5) Bailey, A., Johann, J., & Kang, H.K. (2017). Cognitive and Physiological Impacts of Adventure Activities: Beyond Self-Report. *Journal of Experiential Education 40* (2), 153-169.

Other Products

1) [INVITED] Bailey, A. & Kang H.K. (2019) Tracking and optimizing recreational experiences with biofeedback. Conference of Righteous Sports Culture and Olympics in Korea, Seoul National University, South Korea; August 2019.
2) [INVITED] Bailey, A. (2019). Improving attention in public schools through Riding For Focus. The Specialized Foundation annual research conference, Stanford University; July 2019.
3) Bailey, A., Lewis, T.G., & Kang, H.K. (2017). Adventure Tourism and Outdoor Recreation: Unique but allied industries. *Journal of Outdoor Education, Recreation, & Leadership* 9(2), 244-247.
4) Bailey, A. & Russell, K (2012). Volunteer Tourism: Powerful programs or predisposed participants? *Journal of Hospitality and Tourism Management, 19*, e12.

5) Bailey, A. W., Allen, G., Herndon, J., & Demastus, C. (2018). Cognitive benefits of walking in natural versus built environments. *World Leisure Journal*, *0*(0), 1–13. https://doi.org/10.1080/16078055.2018.1445025

(d) ***Synergistic Activities***

1. Chattanooga Marathon Brainwave Project. Award from the City of Chattanooga and Chattanooga Sports Committee to highlight innovation through EEG activity monitoring during the Chattanooga Marathon (2016-2018, total funding $25,000). Partners included: City of Chattanooga, Chattanooga Sports Committee, EPB of Chattanooga, Blue Cross/Blue Shield of TN, CarbonFive tech Co.
2. Founded the UTC Tourism Center (https://www.utc.edu/health-human-performance/tourism-center.php). Produce research on regional economic, social, and environmental impacts of tourism. Partnerships include: Chattanooga Sports Committee, Hamilton County Government, Chattanooga Department of Transportation, and various non-profits (Chattanooga Zoo, RiverRocks, Riverbend Festival, etc).
3. Cumberland Trail Conference research (2016-2018). In conjunction with the Environmental Science Department, this award of $60,000 supported two Graduate Assistants (1 HHP & 1 ES) for two years to plan the expansion of the Cumberland trail. Senior Principal Investigator: Dr. Jennifer Boyd (2016-2018).
4. High-Impact Grant awards (totaling >$14,000) for design, construction, and research on outdoor learning spaces for Red Bank, Rivermont, and Gilbert Elementary Schools (2016-2018). Partners included: Hamilton County Parks, Hamilton County Dept. of Education, Walker County Schools (GA), and Southeastern Conservation Corps.
5. Consultant for Hamilton County Parks and City of Chattanooga Mayoral Committee. Produced reports for the County Mayor regarding green space priorities (https://www.utc.edu/health-human-performance/pdfs/hcpword.pdf) and served on the Sports and Outdoors Committee for the mayor's Chattanooga Forward Initiative (http://www.chattanooga.gov/images/citymedia/mayorsoffice/CHA%20FWD%20Sports%20&%20Outdoors%20Task%20Force%20Report.pdf).

(d) ***Student Research Advisor/Thesis Committees (100+ annual advisees, 30+ undergraduate research publications/presentations*, 10+ graduate student publications/presentations, Multiple DHON theses)***

- Cox, G. & **Bailey, A**. (2018)*. Comparative analysis of EEG-based mental states in urban environments and green spaces. Presentation for the Southeastern Recreation Research Conference (SERR), Athens, GA; March 2018.
- Somers, M., Locke, J.B., and **Bailey, A**. (2017)*. Analysis of Brainwave data in Outdoor Education. Presentation for the Southeast Regional conference for the Association for Experiential Education: Black Mountain, NC; April, 2017.
- Eastlick, M., Hardin, J., & **Bailey, A**. (2016)*. Adventure Tourism: Understanding Climbing Advocates in Chattanooga, TN. Presentation for NCUR: Asheville, NC; April 2016.
- McDowell, A., Mihalczo, A., and **Bailey, A**. (2016)*. Economic impact of climbing in Chattanooga: A look at the Triple Crown Bouldering competition. Presentation for National Conference for Undergraduate Research (NCUR): Asheville, NC; April 2016.
- Bailey, A., Greganti, C., Hein, K. (*In Review*)*. Randomized control study of a public school forest kindergarten. . *Journal of Educational Research.*
- Hill, S. & **Bailey, A.** (2014)*. Adventure Tourism: Impacts of Tourists at RiverRocks Outdoor Festival. Poster presentation for UTC Research Day, April, 2014.
- Welch, A. & **Bailey, A**. (2013)*. Parks & Green Space Planning: Hamilton County Action Research. Poster Presentation for UTC Research Day, April, 2013.

Biographical Sketch

Vahid Disfani

University of Tennessee at Chattanooga

Department of Electrical Engineering

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(a) Professional Preparation

Undergraduate	Amirkabir University of Technology, Iran	Electrical Engineering	B.S. 2006
Graduate	Sharif University of Technology, Iran	Electrical Engineering	M.S. 20018
Graduate	University of South Florida	Electrical Engineering	Ph.D. 2015

(b) Appointments

2017 – Present	University of Tennessee at Chattanooga, Assistant Professor
2015 – 2017	University of California San Diego, Postdoctoral Scholar
2012 – 2015	University of South Florida, Graduate Research/Teaching Assistant

(c) Publications

(i) Most Closely Related Products

1. Disfani, V.R., Fan, L., Piyasinghe, L. and Miao, Z., **2014**. Multi-Agent Control of Community and Utility Using Lagrangian Relaxation Based Dual Decomposition. Electric Power Systems Research, 110, pp.45-54.
2. Li, C., Disfani, V.R., Pecenak, Z.K., Mohajeryami, S. and Kleissl, J., **2018**. Optimal OLTC voltage control scheme to enable high solar penetrations. Electric Power Systems Research, 160, pp.318-326.
3. Babacan, O., Ratnam, E., Disfani, V.R., and Kleissl, J., **2017**. Distributed Energy Storage System Scheduling Considering Tariff Structure, Energy Arbitrage and Solar PV Penetration. Solar Energy.
4. Disfani, V.R., Fan, L. and Miao, Z., **2015**, July. Distributed DC Optimal Power Flow for Radial Networks Through Partial Primal Dual Algorithm. In 2015 IEEE Power & Energy Society General Meeting. IEEE.
5. Khazaei, J., Piyasinghe, L., Disfani, V.R., Miao, Z., Fan, L. and Gurlaskie, G., **2015**, July. Real-Time Simulation and Hardware-In-the-Loop Tests of a Battery System. In 2015 IEEE Power & Energy Society General Meeting. IEEE.
6. Khorani, V., Razavi, F. and Disfani, V.R., **2011**. A Mathematical Model for Urban Traffic and Traffic Optimization Using a Developed ICA Technique. IEEE Transactions on Intelligent Transportation Systems, 12(4), pp.1024-1036.

(d) Synergistic Activities

- **Interdisciplinary research approach**. Dr. Disfani's research involves power system optimizations, grid integration of distributed energy resources, and Smart Grids. One current research project on development of an urban electric vehicle charging market is in collaboration with the College of Business and the Departments of Computer Science and Engineering at the University of Tennessee at Chattanooga (UTC), and has attracted an internal award funded by UTC SimCenter. This project aims to simultaneously (1) maximize the social welfare among owners of EVs and EV charging stations, and (2) minimize fuel consumption, wasted time, and environmental emissions.

- **Local industry collaboration**. Dr. Disfani collaborated with local industry partners, including TVA and EPB. He also has an active research project funded by TVA.
- **Curriculum development**. Dr. Disfani has developed a graduate level course on power system optimization and smart grids with focus on distributed optimization techniques and grid integration of distributed energy resources including electric vehicles.
- **Community outreach**. Dr. Disfani seeks to engage local high school and community college students in electrical engineering through the development of an online interface for the electric vehicle charging market design through his active grant. The web-based platform will be used to increase public knowledge of EVs and EV charging process and to promote using electric vehicles for less environmental emissions.

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

2014-present	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, co-authoring 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.

Gregory W. Heath, DHSc, MPH

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A. Professional Preparation

Westmont College	Santa Barbara, CA	Psychology	B.A., 1972
Loma Linda University	Loma Linda, CA	Epidemiology	M.P.H., 1977
Loma Linda University	Loma Linda, CA	Physiology/Nutrition	D.H.Sc., 1977
Washington University	St. Louis, MO	Applied Physiology NIH-Post-Doc,	1977-79
Centers for Disease Control (CDC)	Atlanta, GA	Epidemic Intelligence Service	1985-87

B. Appointments

2005–present **Guerry Professor and Assistant Vice Chancellor for Research**
University of Tennessee at Chattanooga, Dept. of Health and Human Performance, Chattanooga, TN, USA

2005–Present **Professor**
University of Tennessee College of Medicine Chattanooga, Dept. of Internal Medicine Chattanooga, TN, USA

2000–2005 **Lead Health Scientist**
Centers for Disease Control and Prevention, Division of Nutrition, Physical Activity, Obesity
Atlanta, GA, USA

1987–2000 **Epidemiologist/physiologist**
Centers for Disease Control and Prevention, National Center for Chronic Disease Prevention and Health Promotion
Atlanta, GA USA

1985-1987 **Epidemic Intelligence Service Officer (EISO),** Centers for Disease Control and Prevention, Center for Health Promotion and Education
Atlanta, GA

C. Products

Products Most Closely Related to Proposal

[1] **Heath GW** and Bilderback J. Grow Healthy Together: Effects of policy and environmental interventions on physical activity among urban children and youth. *Journal of Physical Activity and Health*. 2019; 16:172-176.

[2] **Heath GW**, Parra DC, Sarmiento OL, Andersen LB, Owen N, Goenka S, Montes F, Brownson RC. Evidence-based intervention in physical activity: lessons from around the world. Lancet 2012; 380:272-81.

[3] Sallis JF, Bull F, Guthold R, **Heath GW**, et al. Physical Activity 2016: Progress and Challenges: Progress in physical activity over the Olympic quadrennium. Lancet. 2016 Jul 27. pii: S0140-6736(16)30581-5. doi: 10.1016/S0140-6736(16)30581-5.

[4] **Heath GW**, Brownson RC, Kruger J, Miles R, Powell KE, Ramsey LT. The Effectiveness of Urban Design and Land Use and Transport Policies and Practices to Increase Physical Activity: A Systematic Review. Journal of Physical Activity and Health. 2006; 1:S55-S71.

[5] Bassett DR, Fitzhugh EC, **Heath GW**, et al. Estimated energy expenditures for school-based policies and active living. Am J Prev Med. 2013;44(2):108–113.

Other Significant Products

[1] Fulton JE, Carlson SA, Ainsworth BE, Berrigan D, Carlson C, Dorn JM, **Heath, GW**, et al. Strategic Priorities for Physical Activity Surveillance in the United States. *MSSE*. 2016; 48(10):2057-69.

[2] Varela AR, Pratt M, Powell K, Lee IM, Bauman A, **Heath G**, Martins RC, Kohl H, Hallal PC. Worldwide Surveillance, Policy, and Research on Physical Activity and Health: The Global Observatory for Physical Activity. J Phys Act Health. 2017 Sep;14(9):701-709.

[3] **Heath GW**, Troped PJ. The role of the built environment in shaping the health behaviors of physical activity and healthy eating for cardiovascular health. Future Cardiology 2012; 8(5):677-9.

[4] Lee IM, Bauman AE, Blair SN, **Heath GW**, Kohl HW 3rd, Pratt M, Hallal PC. Annual deaths attributable to physical inactivity: whither the missing 2 million? Lancet. 2013 Mar 23; 381(9871):992-3.

[5] **Heath GW**. The Role of the Public Health Sector in Promoting Physical Activity: National, State, and Local Applications. J Phys Act Health. 2009 Nov;6 Suppl 2: S159-67.

Complete List of Published Work in MyBibliography:
https://www.ncbi.nlm.nih.gov/myncbi/gregory.heath.1/bibliography/public/

Synergistic Activities

Developed public health curricula with focus on active living research

In my first 2 years of appointment I developed graduate courses in introduction to epidemiologic methods; physical activity epidemiology; health behavior change; introduction to biostatistics; How Should We Live: A Quantitative Perspective.

Community Services

American Heart Association, Chattanooga Chapter Board of Directors (2007-2010)

Science Advisor: Grow Healthy Together Chattanooga, Chattanooga/Hamilton County Health Dept

Southside Community Health Coalition – Member (current)

Board of Directors, Lifespring Community Health (clinic and health advocacy)

Professional Services

National:

- Chair, Science Board, President's Council on Fitness, Sports, and Nutrition – 2009-2012
- National Cancer Institute Participatory Research on Cancer Prevention – Advisory Committee
- Institute of Medicine (IOM) – Moderator for Physical Activity and Health Guidelines – 2006
- Journal of Physical Activity and Health – Editorial Review Board
- American College of Sports Medicine – Vice President (2008-2011); Trustee (1996-1999); Chair, Exercise is Medicine Science Committee (2013-2016)

Regional:

- Southeast Tennessee Regional Health Board Member (current)
- Governor's Council on Physical Fitness and Health – Member (2005-2010)

Awards

- Delta Omega, Kappa Chapter (Honorary Public Health Society)
- Charles C. Shepard Science Award, Prevention and Control (Centers for Disease Control and Prevention): "Cost Effectiveness of Community-based Physical Activity Interventions" (2009).
- Elected to Alpha Society, University of Tennessee at Chattanooga Academic Honor Society (2006)

Hamdy Ibrahim
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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.

Charlie Mix
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(a) Professional Preparation

Jacksonville State University	Jacksonville, Alabama	Geography	Bachelor of Science 2009

(b) Appointments

2018- Present	Geographic Information Systems (GIS) Director, University of Tennessee Chattanooga, Chattanooga, TN, USA
2015 - 2018	Geographic Information Systems (GIS) Manager, University of Tennessee Chattanooga, Chattanooga, TN, USA
2013 – 2014	Interim Executive Director, North Chickamauga Creek Conservancy, Hixson, TN US

2013 – 2014	Interim Executive Director, North Chickamauga Creek Conservancy, Hixson, TN US
2012 -2014	GIS Coordinator, North Chickamauga Creek Conservancy, Hixson, TN, USA

2011 – 2012	Park Guide, National Park Service-Chickamauga and Chattanooga, Fort Oglethorpe, GA, USA

2010 – 2011	Conservation Planner, North Alabama & Georgia Land Trust, Piedmont, AL, USA
2010 - 2011	Research Assistant, National Park Service-Russell Cave National Monument, Bridgeport, AL, USA

(c) Products

1. **2017 Habitat Core and Corridor Modeling**

While working on the Thrive 2055 Chattanooga Regional planning project, I created a new geospatial model for environmental conservation of the region. I mapped and ranked forested areas 25 acres or greater that can protect the biodiversity of species and ecosystems for the 16-county region of Chattanooga, TN. The model ranks areas on a 1-5 scale of importance using soil diversity, abundance of wetlands, mileage of streams, the number of ecosystems, the number of known listed endangered or threatened species, and the thickness of the cores. After the cores were mapped and identified, a least cost path analysis avoiding major roads and towns identified all possible connections, enabling us to map potential wildlife corridors: an important network that allows the genetic flow of species through the region. These data are critical for the identification and ranking of local geographic areas for environmental conservation projects by city and regional planners and conservation practitioners in the region. This data can be seen at:

https://congeo.maps.arcgis.com/apps/Styler/index.html?appid=591f643addb5474c9ab321d80a00543c

2. **2017 3D Mapping of Chattanooga, TN**
   Using Light Detection and Ranging Data (Lider) data collected from Tennessee's Lidar program, I mapped over 5000 residential and commercial buildings in downtown Chattanooga creating a 3D map that provides building height and roof type. This information is used in maps analyzing the skyline of Chattanooga and how it might be impacted by future developments. This data can be seen at:
   https://congeo.maps.arcgis.com/home/webscene/viewer.html?webscene=b865ae185c5a41db904b9f5bba4b31a4
3. **2017-2018 Mainspring Conservation Trust**- As principle investigator, I developed a priority conservation model and web mapping tool for Mainspring Conservation Trust, a land trust dedicated to the conservation of the Little Tennessee and Hiwassee River watersheds. In partnership with Mainspring, we developed models that map terrestrial habitat, water resources, recreation and scenic areas, and historic and cultural areas from over 90 layers of data. These models provided an estimated conservation value of the land. Following model optimization, we developed a custom GeoPlanner for the ArcGIS application that enables Mainspring to identify focus areas and prioritize projects for conservation and restoration. These data and tools are used daily by Mainspring staff to guide conservation efforts for one of the most biodiverse and culturally rich regions in the United States.
4. **2019 Mainspring Conservation Trust Priorities cartographic map**. This print map won 3rd place at the 2018 Esri International GIS User Conference and is being published in Esri Map Book, Volume 34, scheduled for publishing in July, 2019. https://mapgallery.esri.com/map-detail/5b0f577674204e43b4a230fb

(d) Synergistic Activities

1. **2015-present -Thrive Regional Partnership**- As the principle investigator, I provided GIS support performing spatial analysis and cartography related to Transportation, Conservation, Economic Development of the greater Chattanooga, TN region. As part of this project, I've also been responsible for cartography and web mapping application development.
2. **2016-2018- Cumberland Trails Conference**- As co-principle investigator, I collected, processed, analyzed and created cartographic maps and web applications pertaining to possible routes/corridor that connect the Cumberland Trail, a long distance hiking trail stretching from Chattanooga, TN to the Kentucky Boarder along the Cumberland Plateau, to communities and other existing trail systems. This work involved supervising and mentoring graduate students and volunteers who were aiding in the work.
3. **2018 Spatial Analysis and Mapping of Historic Tax Data for Chattanooga, Tennessee**- As principle investigator, I mapped and performed spatial analysis of historic property tax records provided by the Enterprise Center for downtown Chattanooga and Hamilton County, TN for the years of 1993-2017. The purpose of this project was to measure and visualize the economic growth of Chattanooga land parcels, demonstrating the economic expansion of Chattanooga.
4. **2018** Presented by invitation at the Esri Federal GIS Users Conference in Washington D.C. on developing web applications for landscape conservation planners.
5. **2018** Presented by invitation at the Esri Geodesign Summit at Esri's headquarters in
6. Redland's, CA on developing web applications for landscape conservation planners.

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
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

Five publications most closely related to the proposed project

1. 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

2. 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

3. Panagiotou E. and Kröger M., 2014, Pulling force-induced elongation and alignment effects on entanglement and knotting characteristics of linear polymers in a melt *Phys. Rev. E* **90** 042602.

4. Panagiotou E., Kröger M and Millett K. C., 2013, Writhe and mutual entanglement combine to give the entanglement length *Phys. Rev. E* **88** 062604.

5. Panagiotou E., Tzoumanekas C., Lambropoulou S., Millett K. C. and Theodorou D. N., 2011, A study of the entanglement in systems with periodic boundary conditions *Prog. Theor. Phys. Supplement* **191** pp.172-181

Five other significant publications

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

2. Panagiotou E. and Plaxco, W. K., 2018, A topological study of protein folding kinetics *Topology of Biopolymers, AMS Contemporary Mathematics Series* (accepted)

3. Panagiotou E. and Millett K. C., 2018, Linking matrices in systems with periodic boundary conditions *J. Phys. A: Math. Theor.*, **51** 225001

4. Igram S., Millett K. C. and Panagiotou E., 2016, Resolving critical degrees of entanglement in olympic rings systems, *J. Knot Theory Ramif.* **25** 14, 1650081.

5. Panagiotou E., Millett K. C. and Lambropoulou S, 2010, The mean squared linking number and the writhe of uniform random walks in confined space *J. Phys. A:Math. Theor.* **43** 045208-30.

Synergistic Activities

1. Organization of AMS meeting: October 10-11, 2020 (Saturday - Sunday) University of Tennessee at Chattanooga, Chattanooga, TN (AMS Fall Southeastern Sectional Meeting) Meeting 1161

2. summer 2014, summer 2015 Co-supervision of research program of Leticia Flores, CAMP (California Alliance for Minority Participation) summer undergraduate research program at the Materials Research Laboratory UCSB

3. Participation in project "Liquid crystals with applications to biology, in MCAIM-WIMM (Women in Mathematics of Materials) Workshop, University of Michigan, Ann Arbor, May 14-18, 2018

4. Participation in "Paths to Collaboration with Scientists", Panel Discussion on behalf of the Committee on the Profession of the AMS, JMM, San Diego, January 10-13, 2018

5. Special talks: "The linking number in systems of curves with Periodic Boundary Conditions", in the Hypatian Seminar, (Women association), UCSB, May, 05, 2014

Reetesh Ranjan
Assistant Professor
Department of Mechanical Engineering
University of Tennessee at Chattanooga
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(a) Professional Preparation

Indian Institute of Technology	Kanpur, India	Mechanical Engineering	B Tech (2004)
University of Illinois	Urbana-Champaign, IL	Theoretical & Applied Mechanics	MS (2009), PhD (2012)
Georgia Institute of Technology	Atlanta, GA	Aerospace Engineering	2013-2015

(b) Appointments

Assistant Professor, University of Tennessee at Chattanooga, 8/2019-till date
Senior Research Engineer, School of Aerospace Engineering, Georgia Institute of Technology, 7/2019
Research Engineer II, School of Aerospace Engineering, Georgia Institute of Technology, 7/2015-6/2019
Postdoctoral Fellow, School of Aerospace Engineering, Georgia Institute of Technology, 1/2013-7/2015
Graduate Research Assistant, Mechanical Science & Engineering, University of Illinois, 8/2007-12/2012
Lead Application Engineer, Ansys India, 7/2004-7/2007

(c) Products

(i) Ranjan, R., Muralidharan, B., Nagaoka, Y., & Menon, S. (2016). Subgrid-scale modeling of reaction-diffusion and scalar transport in turbulent premixed flames. *Combustion Science and Technology*, *188*(9), 1496-1537. https://doi.org/10.1080/00102202.2016.1198336

(ii) Ranjan, R., Panchal, A., Hannebique, G., & Menon, S. (2016). Towards numerical prediction of jet fuels sensitivity of flame dynamics in a swirl spray combustion system. In *52nd AIAA/SAE/ASEE Joint Propulsion Conference* (p. 4895). https://doi.org/10.2514/6.2016-4895

(iii) Ranjan, R., & Menon, S. (2017). Numerical investigation of structural and statistical features of premixed flame under intense turbulence. In *TSFP DIGITAL LIBRARY ONLINE*. Begel House Inc. http://tsfp10.org/TSFP10_program/1/309.pdf

(iv) Srinivasan, S., Ranjan, R., & Menon, S. (2015). Flame dynamics during combustion instability in a high-pressure, shear-coaxial injector combustor. *Flow, Turbulence and Combustion*, *94*(1), 237-262. https://doi.org/10.1007/s10494-014-9569-x

(v) Panchal, A., Ranjan, R., & Menon, S. (2019). A Comparison of Finite-Rate Kinetics and Flamelet-Generated Manifold Using a Multiscale Modeling Framework for Turbulent Premixed Combustion. *Combustion Science and Technology*, 1-35. https://www.tandfonline.com/doi/abs/10.1080/00102202.2019.1580701

(vi) Ochs, B., Ranjan, R., Ranjan, D., & Menon, S. (2019). Topology and flame speeds of turbulent premixed flame kernels in supersonic flows, Combustion and Flame, 210, 83-99. https://doi.org/10.1016/j.combustflame.2019.07.029

(vii) Gonzalez-Juez, E. D., Kerstein, A. R., Ranjan, R., & Menon, S. (2017). Advances and challenges in modeling high-speed turbulent combustion in propulsion systems. *Progress in Energy and Combustion Science*, *60*, 26-67. https://doi.org/10.1016/j.pecs.2016.12.003

(viii) Yang, S., Ranjan, R., Yang, V., Menon, S., & Sun, W. (2017). Parallel on-the-fly adaptive kinetics in direct numerical simulation of turbulent premixed flame. *Proceedings of the Combustion Institute*, *36*(2), 2025-2032. https://doi.org/10.1016/j.proci.2016.07.021

(ix) Ranjan, R., Pantano, C., & Fischer, P. (2010). Direct simulation of turbulent swept flow over a wire in a channel. *Journal of Fluid Mechanics*, *651*, 165-209. https://doi.org/10.1017/S0022112009993958

(x) Ranjan, R., & Pantano, C. (2013). A collocated method for the incompressible Navier–Stokes equations inspired by the Box scheme. *Journal of Computational Physics*, *232*(1), 346-382. https://doi.org/10.1016/j.jcp.2012.08.021

(d) Synergistic Activities

(i) **Novel Computational Methodologies & Algorithms:** The PI has worked on development and application of high-fidelity numerical approaches, which has led to solvers such as *BoxNS* (a parallel incompressible flow solver with discretely mimetic properties) and *CoolSim* (a state-of-the-art tool for investigation of flow and heat transfer in data-center facilities). In addition, the PI has contributed to development and modernization of *AVF-LESLIE* (a compressible reacting flow solver) and *MINCLES* (a multi-scale incompressible flow solver), further development and management of *LESLIE* (a multiphysics tool), and *PRISM* (a spectral element based incompressible flow solver).

(ii) **Creation, Integration & Transfer of Knowledge:** While working in the Computational Combustion Laboratory at Georgia Tech, the PI established several collaborative and documentation strategies by using TRAC and Sphinx tools for efficient transfer of knowledge to students, development of databases, and establishment of best practices.

(iii) **Development & Refinement of Research Tools:** The PI was involved in the development and modernization of *AVF-LESLIE*, a combustion simulation code, which reached a milestone for *in situ* visualizations to achieve "*extreme scale knowledge discovery*". The accomplishment was credited to the expertise of the collaborators, which included Intelligent Light Inc., Georgia Tech and Lawrence Berkeley National Laboratory with funding from the Department of Energy.

(iv) **Service to Scientific & Engineering Community:** *Reviewer* of several archival publications (Flow Turbulence & Combustion, Combustion Theory & Modeling, Computer & Fluids, J. of Propulsion & Power, Physics of Fluids, Shock Waves, I. J. of Heat & Mass Transfer, I. J. of Numerical Methods in Fluids, The Aeronautical Journal, J. of Process in Mechanical Engineering, ASME Turbo Expo, DOE ALCC), *Session chair at conferences* (APS DFD (2013, 2018), AIAA SciTech (2014, 2015), AIAA JPC (2018)), and *Judge* (Georgia Science & Engineering Fair (2016))

(v) **Mentorship Activities:** The PI has mentored 2 high-school students and 10 undergraduate students on the use of computational methodologies to solve fluids and combustion problems, guided 12 graduate students in their thesis related research, and co-advised 1 graduate student. These students belonged to a broad background.

Dr. Yunye Shi

Department of Mechanical Engineering, University of Tennessee in Chattanooga, e-mail: Yunye-Shi@utc.edu,

(a) Professional Preparation

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, IA; Mechanical Engineering; Ph.D., 2016

(b) Appointments

2015–present: **Assistant Professor**, St. Ambrose University, Davenport, IA

(c) Products

1. Zang, G., Jia, J., **Shi, Y.**, Sharma, T., Ratner, A. Modeling and economic analysis of waste tire gasification in fluidized and fix bed gasifiers. *Waste Mangement*. 2019.
2. **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. In: *ASME 2018 International Mechanical Engineering Congress and Exposition*. 2018.
3. Sharma, T., Maya, D., Nascimento, R., **Shi, Y.**, Ratner, A., Lora, E., Mendes, L., Palacios, J., An Experimental and theoretical study of the gasification of miscanthus briquettes in a double-stage downdraft gasifier: syngas, tar and biochar characterization. *Energies*. 2018.
4. 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. In: *American Society for Engineering Education 2018 Conference Proceedings*, 2018.
5. **Shi, Y.**, Sharma, T., Ratner, A. Biomass gasification in a pilot-scale gasifier. In: *ASME 2014 International Mechanical Engineering Congress and Exposition*. 2014.
6. **Shi, Y.**, Sharma, T., Ratner, A., Characterization of real time producer gas generation from paper sludge gasification. *ASME 2013 International Mechanical Engineering Congress and Exposition*. 2013.
7. 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

1. **Conference service:** (i) Topic organizer for combustion mini-symposium session "bioenergy and biofuel", ASME International Mechanical Engineering Congress, Salt Lake City, UT, 2019. (ii) Topic organizer for combustion mini-symposium session "bioenergy and biofuel", ASME International Mechanical Engineering Congress, Pittsburgh, PA, 2018. (iii) Reviewer for ASME International Mechanical Engineering Congress, 2018-2020.
2. **University service:** (i) Chair of committee for Faculty Development, 2019-2020. (ii) Reviewer of St. Ambrose University Undergraduate Research Conference, 2017-2018.

3. **Community service:** (i) Chair of Sigma Xi John Deere Chapter, 2018-2019 (ii) Reviewer of Junior Academy Research Proposals, Iowa Academy of Science, 2018 (iii) Panelist, NSF GRFP Review, 2018, 2019.
4. **Mentoring:** (i) Faculty adviser for Undergraduate Research Program at St. Ambrose University, 2016-2019. (ii) Faculty mentor of St. Ambrose University Summer Research Program, St. Ambrose University, 2018.

(e) Collaborators & Other Affiliations

Collaborators and Co-Editors: *The University of Iowa*: Albert Ratner; Tejasvi Sharma; Guiyan Zang; *The Federal University of Itajuba*: Diego Yepes; Electo Silva;

Biographical Sketch – Craig Tanis

(a) Professional Preparation

Tulane University	New Orleans, LA	Computer Engineering	BSE 1997
Tulane University	New Orleans, LA	Computer Science	MS 1998
University of Tennessee	Chattanooga, TN	Computational Engineering	PhD 2013

(b) Appointments

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

(c) Products

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

2. Chang Phuong, Noman Saied, Craig Tanis. September 2019. "Assessing Kokkos Performance on Selected Architectures". Latin America High Performance Computing Conference 2019 (Proceedings).

3. Craig Tanis, Kidambi Sreenivas, Robert Webster, James Newman. June 2018. "Performance Portability of a Multiphysics Finite Element Code". AIAA Aviation Forum 2018 (Proceedings).

4. Craig Tanis. December 2013. "A NEW SOFTWARE FRAMEWORK FOR UNSTRUCTURED MESH REPRESENTATION AND MANIPULATION" (Dissertation). https://scholar.utc.edu/theses/89/

5. W. Kyle Anderson, Li Wang, Sagar Kapadia, Craig Tanis, Bruce Hilbert. September 2011. "Petrov-Galerkin and discontinuous-Galerkin methods for time-domain and frequency-domain electromagnetic simulations". Journal of Computational Physics, vol. 230, no 23. pp 8360-8385.

(d) Synergistic Activities

1. XSEDE Campus Champion for UT Chattanooga (2014-Present).

2. XSEDE Campus Champion Fellow (2015-2016).

3. Course developer and teacher of graduate courses on Parallel Programming (CPSC 5260) and High Performance Computing (CPSC 7110).

4. Textbook Reviewer (2017): High Performance Computing: Modern Systems and Practice, by Sterling et. al.

Biographical Sketch

Sungwoo Yang
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(a) Professional Preparation

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

(b) Appointments

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

(c) Publications

(i) Most Closely Related Products

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

(ii) Other Products

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

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

(d) Synergistic Activities

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

Appendix B

Awardee Project Reports

New Projects for FY 2021

Fiscal Year 2021 Final Project Report

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

Dr. Abdollah (Abi) Arabshahi, Lead PI

Co-PI(s): Dr. Reetesh Ranjan
Other Personnel: Timothy Johnston – Graduate Student Researcher

Project Title: Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase Flows

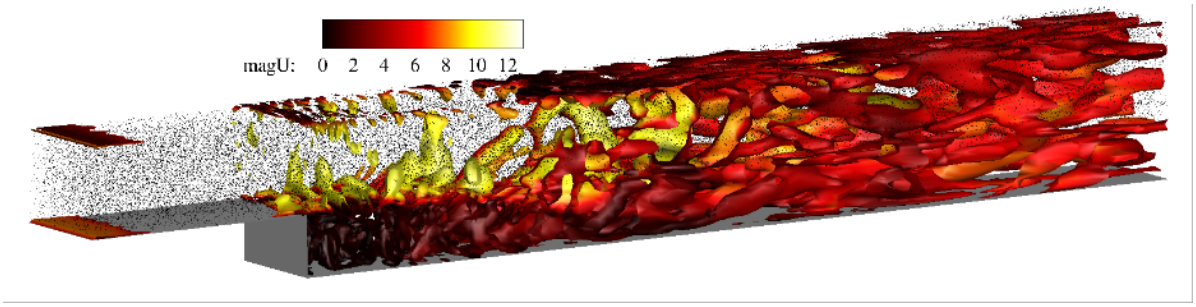
Date Submitted: 07/30/2021

Award Start – End Date: July 1, 2020 – June 30, 2021

Non-Technical Summary:

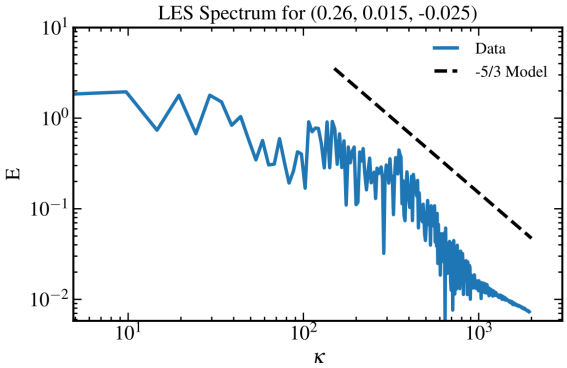
The project was intended to assess particle-laden flows, which are seen in nature and in industrial applications. Understanding more about the dynamics through simulations can improve the numerous applications. Numerical investigation of such flows under practical scenario is typically performed using two well-established approaches, namely, the Eulerian-Lagrangian (EL) formulation, and the Eulerian-Eulerian (EE) formulation, where typically a point-particle assumption is used in both these approaches. The research focused on further enhancements, a comprehensive assessment, and application of the EL framework, where the carrier phase evolution is performed using a Eulerian approach and the dispersed phase is tracked in a Lagrangian manner. Although the EL framework is well-established, there are several challenges associated with the accuracy and the efficiency of this approach, which need to be addressed for improved predictive capabilities. The carrier phase simulation can be performed using direct numerical simulation (DNS), large-eddy simulation (LES), or Reynolds Average Navier-Stokes (RANS) techniques depending upon the required level of fidelity. Here we focused on the EL strategy in the context of LES, which is considered more suitable for engineering applications exhibiting unsteady dynamics. We focused on two key challenges associated with the Lagrangian evolution of the dispersed phase. The first was related to the modeling of the subgrid turbulence dispersion, and the second was related to the use of the notion of parcels for reasons of computational efficiency. Three different subgrid turbulence dispersion modeling strategies were extended and evaluated under the same numerical framework, which include a localized multi-scale two-level simulation (TLS) approach, a fractal interpolation technique (FIT), and an approximate deconvolution (AD) method. To address the accuracy and convergence issues associated with the use of a parcel-based approach, deterministic and stochastic parcel number-density control (PNDC) algorithms were assessed. The enhanced modeling strategies within the EL framework considered in this research effort was verified and validated through well-established test cases.

The thrust was to submit a conference and journal paper, which is still proposed for the end of this year. The student was funded through the grant and the knowledge he obtained is applicable to his master's thesis. He will also be a co-author for the journal and conference articles, which improves his resume and knowledge for his future career. The project supported the mission of the SimCenter by using the advanced computational resources to teach a student as well as producing scholarly outputs. The model will be used in ways that others have not attempted before, so this will be a novel application.



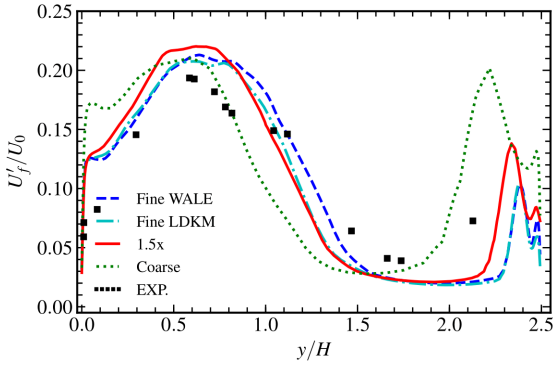
Isosurface showing Q-criterion shaded by particle velocity magnitude, with particles shown as small spheres. The bottom and step walls are shaded for reference.

Energy spectrum spectrum for a step through the -5/3 Model is



plot showing the LES point downstream of the simulation. The Kolmogorov shown for comparison.

PROJECT TITLE: Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase Flows
Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
Particle-laden separating/reattaching flows are studied using the Large-Eddy Simulation (LES) approach with subgrid-scale (SGS) stress tensor and particle dispersion models. • Create a backward-facing step mesh • Perform mesh refinement and scaling studies • Compare SGS stress tensor models without particles • Compare particle dispersion models with a specified mass loading	The student presented work at the 2021 ReSEARCH Dialogues conference, as well as the CECS Technology Symposium. The student will present his thesis in the fall semester. The thrust was to submit a conference and journal paper, which is still proposed for the end of this year.
RESULTS	**OTHER INFO**
Confirmed the computational setup was correct, as the refined mesh cases matched the turbulent velocity fluctuations with models, as shown below. The particle dispersion was compared to the experimental results using a particle number density script, and the results were comparable in the middle x-y plane.  Streamwise velocity fluctuations 5 step-heights downstream from step feature after 24 flow-through times	**Budget and Schedule** Total Budget: $99,221.00 Actual Used: $98,665.46 Balance: $ 555.45 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-6 Task 3: Months 6-12 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication • External and internal conference presentation

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Create a backward-facing step mesh to compare to experimental and previous simulation results.	Created a structured three-dimensional domain that matched the previous simulation setup
Perform scaling mesh analysis to determine optimal number of processors for each case.	Compared the speed-up to increase in processors to determine parallel efficiency
Create LES energy spectrum plot to determine the inertial regime.	Compared to the Kolmogrov -5/3 energy cascade model at different points in the domain
Compare typical LES turbulence models using OpenFoam.	Compared mean and fluctuating velocity components model-to-model and model-to-experimental data, and found WALE to be the most suitable for this application
Test subgrid particle dispersion models on two-way coupled flows.	Tested stochastic and differential filter models on the coarse and fine meshes using 10-20% mass loadings
Implement dynamic procedure for differential filter model based on dissipation matching.	Created model that computes the volume-averaged model parameter dynamically

Challenges & Strategies Used to Address / Overcome:

The student started using an in-house developed solver, but the particle model was not up-to-date. The student switched to OpenFoam due to the community assistance, especially in the Fluids and Combustion Modeling Research Group.

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

The in-house solver was not set up to be used by students and the particle model was not well documented, so the student had much trouble in running the simulations. The goal was to simulate multiple geometries to prove the model's versatility, but only the backward-facing step mesh has been used with a coarse mesh, an intermediate mesh, and a fine mesh. Wall roughness has significant effects on practical flows that need to be modeled somehow, which was not taken into account.

IMPACT & OUTCOMES

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

The research work carried out under this effort will have impacts at various levels on the career of the PI and co-PI in the area of modeling and simulation of particle-laden turbulent flows. The project has helped to assess and evaluate subgrid models for large-eddy simulation (LES) of particle-laden turbulent flows. The extension of the baseline OpenFOAM to the in-house research code referred to as UTCFoam will allow to carry out the study of particle-laden flows in practically

relevant configurations. The UTCFoam has three different types of subgrid dispersion models, which are key for the accurate prediction of particle-laden flows while employing the Eulerian-Lagrangian formulation. The extension and application of the framework to a wide range of flow configurations, such as particle-laden isotropic turbulence, particle-laden separating/reattaching flow, aerosol evolution within the upper human airway, etc., showcases the capabilities within our research group. Overall, the resulting computational capabilities, publications, and presentations will be helpful us in seeking extramural funding.

Students Impacted

Timothy Johnston is in the process of obtaining his master's degree in mechanical engineering. He plans to graduate in the fall semester with his thesis on particle-laden separating/reattaching flows. He was supported with a Graduate Research Assistantship for the Spring Semester of 2020 and has been receiving funding as a temporary research assistant otherwise.

Community and Broader Impacts

Particle-laden turbulent flows are aplenty in nature, as they describe sediment transport in natural systems as well as many mixing processes in combustion chambers. They can also describe granular flow transport in industrial applications, as well as many others. In LES, the subgrid-scale effects of particle motion on the turbulent structures are important to understand. Most practical turbulent particle-laden flows cannot be simulated using DNS, especially wall-bounded flows due the high computational requirements.

Scholarly Products

External Conferences:

The thrust was to submit a conference and journal paper, which is still proposed for the end of this year.

1. Assessment of Subgrid Dispersion Models for Large-Eddy Simulation of Particle-Laden Turbulent Flows, AIAA Scitech, 2021.

Presentations at UTC:

1. 2021 ReSEARCH Dialogues
2. 2021 CECS Technology Symposium

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

- Digital Twins in Production Engineering and High Performance Computing Education Workshop, December 3rd & 4th, 2020
- Established a collaborative research activity with Dr. Dan E. Olson (Professor of Medicine, University of Toledo College of Medicine, MD, PhD, DIC) to explore the potential effect of the COVID-19 virus to create a highly transmittable infection research collaboration, January, 2021

- Established a collaborative research activity with Dr. J. Sethi (Professor of Medicine, Chief of Pulmonary, Critical Care and Sleep Medicine, UTCOM-Erlanger Hospital and Health System) to explore collaborative research activities for patients infected with the COVID-19 in the upper pulmonary airway, Chattanooga, TN, November, 2020
- Research collaboration Dr. Reetesh Ranjan from Mechanical Engineering on the development of a new model for subgrid dispersion of heavy-particles in turbulent particle-laden flows using Large Eddy Simulations
- Research collaboration with Dr. Sou Palchoudhury from Civil & Chemical Engineering on development and applications of a novel computational analysis method to predict the concentration of nanoparticles for the SARS-CoV-2 detection assay for reliable detection sensitivity
- Research collaboration with Dr. Morgan Smith from Anthropology and Dr. Boris Belinskiy from Mathematics on application of a numerical model of low-frequency acoustic wave interaction with stone tools and development of a code for simulating this interaction to identify submerged pre-contact archaeological sites
- Established a collaborative research activity with Dr. Ashley Manning-Berg from Biology, Geology and Environmental Science to develop and perform numerical modeling to predict the range of preserved microbial morphologies given a specific length of time that the microbes were exposed to decomposition

EXTERNAL FUNDING

Proposal Submissions

1. Research proposal entitled, "COVID-19-Patient-Specific HPC Simulation of Pulmonary Airflow Structure and Aerosol Particles Transport/Deposition Patterns," to the IBM Faculty Award Technical Discovery, PI, $50,000, target submission March 2021.
2. Research proposal white paper entitled, "High-Performance Numerical Simulation of Flow Structures and Transport/Deposition of Particles in Pulmonary Airways in Support of COVID-19 treatments in hospitalized and long-haul patients," submitted to the National Science Foundation's Leadership Class Computing Facility (NSF's LCCF), PI, $120,000 - $150,000 per year, February 26, 2021.
3. UT Biomedical Research Initiation Collaborative Grants, "Computational Investigation of Region Aerosol Deposition in Realistic Human Airways," Co-PI, $24,920, January 1, 2020 to December 31, 2020.
4. Department of Energy (DOE), "PSAAP-III (FIC): Center for Understandable, Performant Exascale Communication Systems (CUP-ECS)," Senior Personnel, $1.3M (UTC portion), July 1, 2020 to June 30, 2025.
5. National Science Foundation (NSF), "Collaborative Research: Software Engineering Workforce Development in High Performance Computing for Digital Twins," Co-PI, $57,635, October 1, 2019 to September 30, 2021.
6. National Science Foundation (NSF), "RUI: Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems," PI, $42,269, August 1, 2019 to July 31, 2021.

7. Research proposal white paper entitled, "A Data-Driven Multi-Parameter Reduced Order Modeling Framework for Investigation of Hypersonic Systems," PI, $887,427, AFOSR # FOA-AFRL-AFOSR-2020, 05/01/2021 - 04/30/2024.
8. Research proposal entitled,"COVID-19-Relevant Computational Modeling of Human Respiratory Airways," PI, $1,222,244, PRMPR-IIRA-2020, DOD- Department of the Army, USAMRAA,10/01/2021 - 9/30/2025.
9. Research proposal entitled, "STOP COVID: Stopping Transmission Of airborne Pathogens in Confined spaces Via Integrated Designs," Co-PI, $1,599,432, W81XWH-20-PRMPR-IIRA-COVID, DOD-Department of the Army, USAMRAA, 10/01/2021- 9/30/2025.

Contracts/Awards Received

1. UT Biomedical Research Initiation Collaborative Grants, "Computational Investigation of Region Aerosol Deposition in Realistic Human Airways," Co-PI, $24,920, January 1, 2020 to December 31, 2020.
2. Department of Energy (DOE), "PSAAP-III (FIC): Center for Understandable, Performant Exascale Communication Systems (CUP-ECS)," Senior Personnel, $1.3M (UTC portion), July 1, 2020 to June 30, 2025.
3. National Science Foundation (NSF), “Collaborative Research: Software Engineering Workforce Development in High Performance Computing for Digital Twins,” Co-PI, $57,635, October 1, 2019 to September 30, 2021.
4. National Science Foundation (NSF), “RUI: Efficient Adaptive Backward SDE Methods for Nonlinear Filtering Problems,” PI, $42,269, August 1, 2019 to July 31, 2021.

Sponsored Program Capacity Building Activities

N/A

WHAT’S NEXT FOR THIS RESEARCH?

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

The immediate focus of the PI and co-PI is on the completion of journal articles on the work accomplished during this project. In addition, we will be submitting white papers and proposals, which will leverage the outcomes of the project. In particular, we are planning to pursue three research directions in the next few years. These include (a) development of hybrid stochastic and multi-scale dispersion models, (b) assessing the efficacy of subgrid dispersion models for different levels of inertia of particles, and (c) further extension of the models to spray combustion.

FINANCIAL ACCOUNTING

N/A

Fiscal Year 2021 Final Project Report

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

Yunye Shi, Lead PI

Co-PI(s): none
Other Personnel: none

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

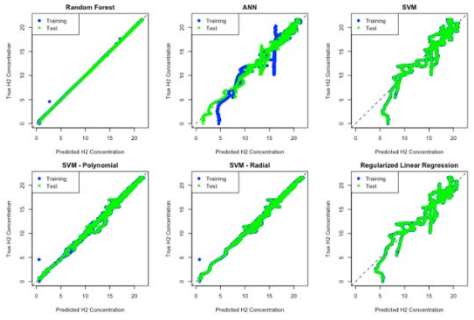
Date Submitted: July 31, 2021

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: Machine Learning Application in Energy Conversion Systems

TECHNICAL APPROACH	OUTCOMES
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.	• The project developed machine learning models that could be used for not only gasification, but other nonlinear processes for future study. • A paper entitled “Predicting Steam-Gasification Output Using Artificial Neural Networks” has been accepted for IMECE 2021 for both publication and conference presentations. • A paper entitled “Predicting Steam-Gasification Output via Machine Learning Approaches” is under review in Energy.
RESULTS	**OTHER INFO**
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. 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. 	**Budget and Schedule** Total Budget: $15,000.00 Actual Used: $ 13,101.33 Balance: $1,898.67 Total period of performance is 12 months. • Task 1: Months 1-4 Data collection and preprocessing • Task 2: Months 4-10 Model building and testing • Task 3: Months10-12 Publication preparation

ACCOMPLISHMENTS & OUTCOMES

Project Overview

<table>
<tr><th>List of Objectives / Aims / Major Milestones Proposed</th><th>Cumulative Outcomes / Accomplishments</th></tr>
<tr><td>Data collection and data preprocessing</td><td>A data base with 16,000 data points was constructed to train models and to test model accuracy.</td></tr>
<tr><td>Random forest model</td><td rowspan="6">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. 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 is an effective method for estimating missing data.</td></tr>
<tr><td>ANN model</td></tr>
<tr><td>SVM model</td></tr>
<tr><td>SVM model with polynomial kernel</td></tr>
<tr><td>SVM model with radial kernel</td></tr>
<tr><td>Regularized regression model</td></tr>
</table>

Challenges & Strategies Used to Address / Overcome:

Since machine learning models need large dataset to train models, one of the challenges is that data collection is time and cost consuming. The data used in the project is collected at the University of Itajuba in Brazil. But due to COVID travel restrictions, data collection can 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 collaboration and enhanced interpersonal communication. This project has sparked many more new ideas between the teams.

Students Impacted

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

Hannah Morgan: Hannah was introduced to the project and conducted basic analysis. Hannah is also pursuing for a master degree at UTC.

Community and Broader Impacts

Biomass utilization is a promising technology to partly replace fossil fuel combustion in power plants. It is environmental friendly in many different aspects CO_2 neutral, less NO_X production and so on. Accurately predicting syngas output not only benefits system design and operation, 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 potentially to be widely used in output prediction in energy conversion processes.

Scholarly Products

1. Paper titled "Predicting Steam-Gasification Output Using Artificial Neural Networks" has been accepted for IMECE 2021 for both publication and conference presentations
2. Paper titled "Predicting Steam-Gasification Output via Machine Learning Approaches" is under review in Energy.

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

1. NSF ERI submitted in 2021 Summer
2. UTC CEACSE submitted in 2020 Fall

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. Several NSF grant webinars
2. 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? What other related research will you pursue (and with whom) in light of the support you've received from CEACSE?

Further work plan has been developed from the current CEACSE project. There are two directions the work will be extended to. One area is to apply the current models to a CFD model for biomass gasification modeling. Another direction is to apply the models to new research questions. Both are further collaboration with the institution in Brazil.

FINANCIAL ACCOUNTING

The leftover grant (around $1800) will be used to continue to support undergraduate student research related to this project.

Fiscal Year 2021 Final Project Report

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

Dr. Vahid Disfani, Lead PI

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

Project Title: Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources

Date Submitted: October 1, 2019

Award Start – End Date: July 1, 2020 – June 30, 2021

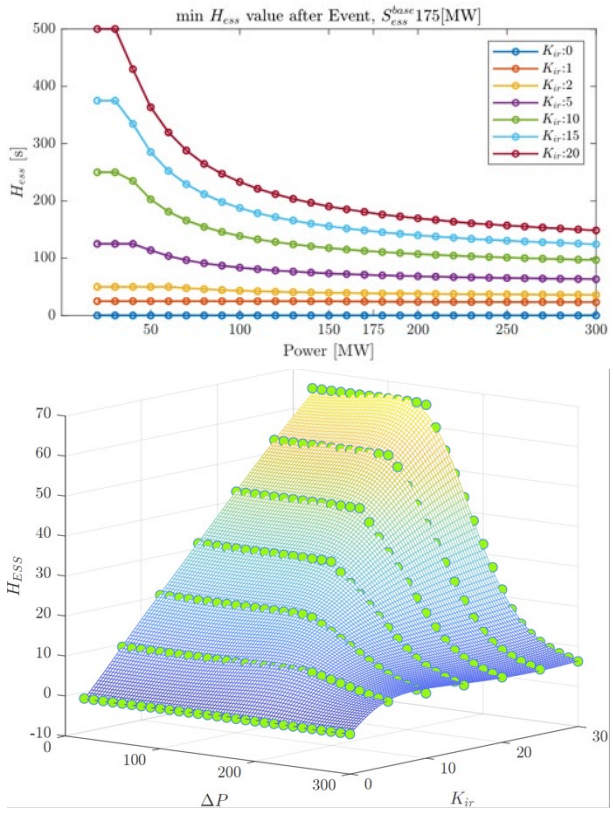
Non-Technical Summary:

Grid integration of high penetration of distributed energy resources is expected to cause serious frequency excursions in power systems. These resources have highly intermittent power output and are connected through zero-inertia power electronic converters, both of which have adverse impacts on power system frequency. The main idea to resolve these issues is to emulate additional inertia through the same converters, which is referred to as virtual inertia. In addition to the total virtual inertia available throughout the power system, its allocation has a significant impact on the frequency behavior of the power systems. This proposed project will develop real-time optimal allocation of virtual inertia in response to real-time forecast for availability of distributed energy resources. Realistic models of virtual inertia by different technologies will be developed. The optimization platform will be finally tested via software and real-time digital simulation platforms.

Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources

Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
To tackle the unexplored research problems, the PIs proposed the following three well-coordinated research tasks for the analysis and design of a real-time solution for optimal VI/VD allocation: • Task 1. Investigating VI and VD Provision of Different DER Technologies • Task 2. Developing Real-Time Adaptive VI/VD Allocation • Task 3. Real-Time Digital Simulation Implementations	2 conference papers: • P. Ubiratan, S. Wasti, and V. Disfani, “Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm,” in 2020 IEEE International Conference on Smart Grid Communications (Smart-GridComm), IEEE, 2020. • P. Ubiratan, S.Wasti, and V. Disfani, “Frequency Deviation Controller for Inter-Area Oscillations Damping in Smart Grids,” in 2021 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT), IEEE, 2021. 1 presentation in UTC ReSEARCH Dialogue • P. Ubiratan, “Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm,” in UTC ReSEARCH Dialogues. 1 MS Thesis • P. Ubiratan, “Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021.

RESULTS	OTHER INFO
	**Budget and Schedule** Total Budget: $92,942.00 Actual Used: $92,942.00 Balance: $ 0.00 Total period of performance is 12 months. Task 1: Months 1-4 Task 2: Months 4-8 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved • Final report detailing results, financials, and future work • Publication • External and internal conference presentation **Organization Information** 615 McCallie Ave., Dept 2342 University of Tennessee at Chattanooga 423-425-4354 Vahid-disfani@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Task 1. Investigating VI and VD Provision of Different DER Technologies	We investigated the positive and negative VI and VD each DER technology can offer. We defined the maximum and minimum VI and VD provided by DERs as functions of their type, nameplate information, power electronics and control interface, and instantaneous operation status. Renewable energy resources (RES), battery energy storage systems (BESS) and ultracapacitors were studied.
Task 2. Developing Real-Time Adaptive VI/VD Allocation	We set up more accurate optimization models for VI and VD allocation using the results of Task 1 and short-term and long-term forecasts RES. Data from Sky Imagers have been obtained from the devices at UC San Diego in this Task.
Task 3. Real-Time Digital Simulation Implementations	We tested the proposed schemes in MATLAB Simulink. We developed software models of auxiliary control systems for different types of DER to provide VI and VD. We then tested them on different power system test cases including IEEE 14-bus, 30-bus, 118-bus, 300-bus.

Challenges & Strategies Used to Address / Overcome:

The main challenge was to get access to short-term solar and wind data. We used UCSD Sky Imager data for solar and some online resources such as http://hint.fm/wind/ for real-time values and short-term forecasts of wind. We obtained access to these datasets during Task 1 to address this risk before we needed them in task 2.

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

One observation that we had throughout the project was that the lack of inertia is much more powerful than the power disturbance of RES when it comes to frequency excursions, while we expected to observe more challenges from power disturbances. The main reason is that power system frequency is a function of total power mismatch in the grid, and the aggregated power from geographically-distributed RESs experiences much lower level of disturbance than the power from each individual RES.

IMPACT & OUTCOMES

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

Dr. Vahid Disfani (PI): This research grant funded through CEACSE helped the PI to make this topic of research one of the research trends in his research. Four master's students collaborated on this project. One M.S. thesis was written as a result of this work.

Dr. Raga Ahmed: Dr. Raga Ahmed was a great help throughout the project by providing outstanding insights on control system designs in Task 2 of the project. This research grant helped Drs. Ahmed and Disfani to build a good collaboration between their research groups for future research.

Students Impacted

Pablo Macedo: Pablo was a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He led Task 1 and 3 of the project. Throughout this project, he learned data processing, data visualization techniques, development of optimization models, and solving them using optimization solvers in MATLAB. Pablo wrote his and defended his M.S. thesis around the topic of this grant. He joined the power system industry in Fall 2021. He authored 2 conference papers from his involvement in this project.

Shailesh Wasti: Shailesh was a master's student and research assistant in Dr. Disfani's research lab in the Electrical Engineering Department. He led Task 2 of the project. Throughout this project, he learned data processing, data visualization techniques, development of optimization models, and solving them using optimization solvers in MATLAB. Shailesh co-authored 2 conference papers from his involvement in this project. Shailesh joined the Pennsylvania State University (PennState) as a PhD student in Fall 2021.

Community and Broader Impacts

The results of this project will enable high penetration of distributed energy resources, especially renewables, on power systems for cheaper electricity and lower carbon emissions. Also, graduate assistants were trained for energy and control careers throughout this project. They leveraged their research capabilities to perform state-of-the-art research in the area of power system control and stability and grid integration of DER.

We also disseminated the results of this project as 2 conference papers, one M.S. thesis, and one UTC ReSEARCH Dialogues presentation. We have reached out to Tennessee Valley Authority to test our algorithms on their power grid.

Scholarly Products

Publications:

1. P. Ubiratan, S. Wasti, and V. Disfani, "Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm," in 2020 IEEE International Conference on Smart Grid Communications (Smart-GridComm), IEEE, 2020.

2. P. Ubiratan, S.Wasti, and V. Disfani, “Frequency Deviation Controller for Inter-Area Oscillations Damping in Smart Grids,” in 2021 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT), IEEE, 2021.
3. P. Ubiratan, “Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021.

External Conferences:

1. P. Ubiratan, S. Wasti, and V. Disfani, “Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm,” in 2020 IEEE International Conference on Smart Grid Communications (Smart-GridComm), IEEE, 2020.
2. P. Ubiratan, S.Wasti, and V. Disfani, “Frequency Deviation Controller for Inter-Area Oscillations Damping in Smart Grids,” in 2021 IEEE Power & Energy Society Innovative Smart Grid Technologies Conference (ISGT), IEEE, 2021.

Presentations at UTC:

1. P. Ubiratan, “Improving Inter-Area Oscillations Damping of Power Systems Through Cooperative Active Power Control of Distributed Energy Resources," at University of Tennessee at Chattanooga, 2021.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

Through this project, we could create some collaborations between UTC, TVA and UCSD. These collaborations are expected to increase in the next rounds of this research.

EXTERNAL FUNDING

Proposal Submissions

1. One NSF CAREER Proposal in July 2020.

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. I attended NSF CAREER workshop set up by NSF in February 2021, after my first submission in 2020.

WHAT'S NEXT FOR THIS RESEARCH?

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

This project will be continued by developing more advanced control and optimization algorithms in short-term. Meanwhile, more open research problems will be identified as basis for more extramural funding proposal submissions in collaboration with TVA.

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

This grant will be followed up by some research projects. More extramural funding proposals will be submitted in collaboration with TVA.

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 2021 Final Project Report

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

Sungwoo Yang, Lead PI

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

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

Date Submitted: 06/30/2021

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

Non-Technical Summary:

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

The project did not have a student researcher due to COVID-19. However, we were able to achieve some proposed milestones: (1) We finalized synthetic method of OTTI aerogel that demonstrated high transmittance (95% solar-weighted). (2) We synthesized ambiently dried aerogel that demonstrated ~ 90% transmittance that is equivalent to the best literature value. As the project is extended, we plan to further improve. (3) We are in progress of developing optical and thermal computational modeling using RTE and Mie theory. (4) We built a lab-scale solar receiver. The PI plans to hire two PhD students to continue this project by using the rollover fund. The goals for the following years are to bring these threads together for research publications and external funding. The PI plans to continue to build a device-level prototype to demonstrate the viability of this approach. The PI plans to submit journal papers including patents. The research progress and products will allow the PI to pursue large funding opportunities, namely the National Science Foundation Faculty Early Career Development (NSF CAREER) award. These research activities are expected to increase the PI's capacity to successfully compete for tenure.

PROJECT TITLE: A Low-Cost, Passive Solar Process Heat System
Technology Area of Interest: Energy Thrust

TECHNICAL APPROACH	OUTCOMES
The major milestones include: 1. Finalized synthetic method of OTTI aerogel 2. Optimizing chemical recipes for ambiently dried aerogel 3. RTE and Mie theory modeling 4. Building solar collector assembly 5. Solar process heat generator design & modeling	The research outcomes include: 1. Won Ruth S. Holmberg Grant 2. Submitted NSF-ERI proposal, $200k (in review) 3. In progress (~50%), a peer-reviewed publication on ambiently-dried aerogel 4. Oral presentation at the Solar Energy Systems Conference (2021)
RESULTS	**OTHER INFO**
Please, see the attached research report for the details	**Budget and Schedule** Total Budget: $86,771.00 Actual Used: $36,167.00 Balance: $50,604.00 **Deliverables** • External funding proposal (submitted) • Final report detailing results, financials, and future work (submitted, and there will be one more final report after the extended year) • Publication (in progress) • External and internal conference presentation (accepted at Solar Energy Systems Conference 2021).

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Chemical recipe for OTTI aerogel	Completed
Optimizing ambiently-dried aerogel	Fabricated. In progress for further improvement
Computational device design optimization	In progress (delayed)
Building solar receiver prototypes	Delayed due to COVID-19, but a lap-scale solar receiver built. Plan to build a larger system for outdoor experiment

Challenges & Strategies Used to Address / Overcome:

- Developing collaboration: The PI aims to develop a novel chemical precursor to synthesize ambiently dried aerogel, which requires deeper chemical understanding. The PI is in progress developing collaboration with faculty members in the Chemistry department at UTC.
- Limited researcher power: the proposed project requires significant amont of efforts to conduct various experiments and theoritical modeling. Limited researcher power is a major challenge the PI has been facing. Especially due to COVID-19, it was extremely difficult to keep researchers. As results, the several milestones were delayed. But, the PI plans to hire two PhD students using the carry over fund for the upcoming semester.

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

As a R3 institute, I found that the CEACSE grant is the most important grant that I can utilize to increase our research capability. Due to the unexpected delay, we were not able to complete all milestones, but plans to complete all in the upcoming semester. I was able to obtain several critical research developments with CEACSE grant. Using these preliminary results, I have submitted multiple proposals and plan to submit more proposals to attract external funding. I really appreciate the CEACSE grant and the supporting team.

IMPACT & OUTCOMES

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

With preliminary data, the PI plans to pursue external funding opportunities related on solar energy harvesting and energy efficient building applications including NSF, NASA, ARPA-e, DARPA and etc. The PI collaborates with Dr. Yang and Dr. Hyatt in Chemistry department at UTC, Dr. Kim in Engineering management at UTC, Dr. Nawaz at the ORNL and Dr. Zhao at 3M.

Students Impacted

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

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

Community and Broader Impacts

With the preliminary result, the PI plans to build a solar grill system which can be used for various outreach events searching prospective students of the Engineering school at UTC.

Scholarly Products

Publications:

1. High Temperature Stable Aerogel by ALD Coating (in revision)
2. Enhanced Solar Receiver Efficiency Using Superhydrophobic Cost-Effective Ambiently Dried Aerogel (in progress, 50%)

External Conferences:

Oral presentation scheduled at the Solar Energy Systems Conference, AIChE, 2021.

Presentations at UTC:

2021 ReSEARCH Dialogues and Technology Symposium

Inventions or Other Intellectual Property

Three patent applications submitted to UTRF.

1. Cheap, strong, waterproof, optically transparent, thermally insulating retrofit
2. Novel Silica Precursor to Synthesize Ambiently Dried Transparent Aerogel
3. Novel Air Burning Method to Synthesize Transparent Insulator

Research Outreach & Collaboration

The PI collaborates with Dr. Yang and Dr. Hyatt in Chemistry department at UTC, Dr. Kim in Engineering management at UTC, Dr. Nawaz at the ORNL and Dr. Zhao at 3M.

EXTERNAL FUNDING

Proposal Submissions

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

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

Contracts/Awards Received

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?

CAREER is the first target. The PI plans to build a research program that last more than 5 years working on the most important problem in the aerogel community.

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

Another major research focus of the PI is aerogel for water harvesting and energy efficient building applications. Transparent insulator, aerogel, can promote both research area.

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

N/A

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

The biggest challenge the PI has been facing is limited researcher power. The PI plan to hire two PhD students for the upcoming year hoping that improves research power. In addition, the PI plan to hire more undergraduate researchers via the URaCE URTOPS Program.

FINANCIAL ACCOUNTING

N/A

CEACSE Program – Final Report on Research Results

The Tasks and Timeline with Milestones/Deliverables

The proposed tasks and timelines are shown below for the 12-month project.

Description \ Month	1	2	3	4	5	6	7	8	9	10	11	12
Finalizing synthetic method of OTTI aerogel (10x10cm2)												
Optimizing chemical recipes for ambient dried aerogel												
Optical & thermal modling via RTE and Mie theory												
Mechanical modeling via molecular dynamics												
Builing solar collector assembly & lab testing												
Solar process heat generator design & modeling												
Constructing the solar process heat generator assembly												
Integrating PCM thermal storage in the heating loop												
Outdoor experiments with the final prototype												
Finalizing commercialization plan and form partnerships												

Research Results

1. Finalizing synthetic method of OTTI aerogel

As shown in Figure 1a, we demonstrated transparent OTTI aerogel with ~ 12 cm diameter. In our lab, we have optimized the silica aerogel fabrication recipe and processing conditions to achieve pore sizes of 2-50 nm. Carefully tailoring the nanostructure of our aerogel samples has allowed us to achieve solar-weighted transmittance greater than 96% for a 3 mm thick sample (Figures 1b) that is the highest transmittance report in the literature. As the gelation reaction (hydrolysis and condensation reactions) is exothermic reaction, the amount of catalyst should be precisely controlled for the scale-up.

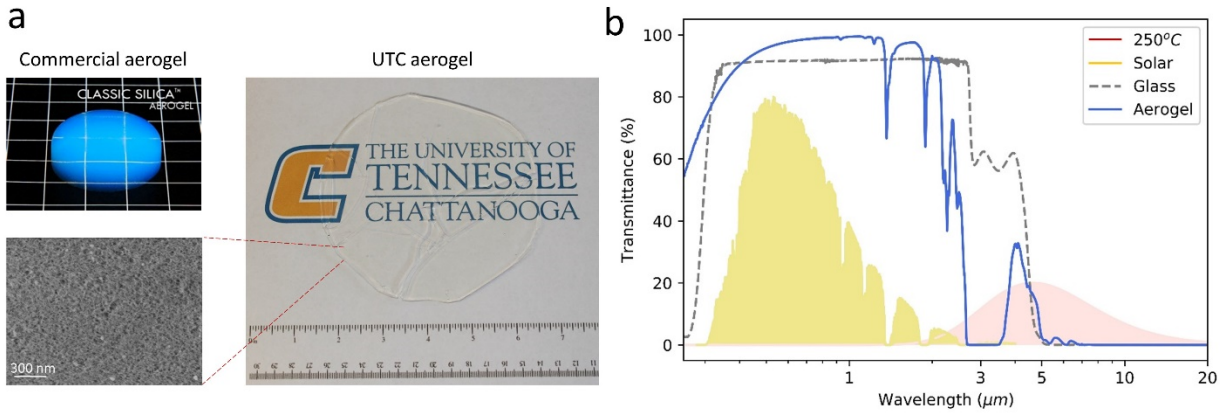


Figure 1: (a-left top) Image of commercially available silica aerogel. (a-right) Image of a 200 mm diameter monolithic silica aerogel sample fabricated in our lab. (c) Measured hemispherical transmittance of the aerogel sample (blue), showing high transparency in the solar spectrum (yellow-filled) and significant suppression of blackbody radiation (red-filled) at the target operating temperature

2. Optimizing chemical recipes for ambiently-dried aerogel

Furthermore, we have reinforced OTTI aerogels via optimizing cross-linked polymers in the aerogels. Improved mechanical properties results in ambient-pressure dried aerogels, which has the potential to greatly reduce the aerogel production cost by an order of magnitude. Figure 2a shows a reinforced ambiently-dried OTTI aerogel. It is superhydrophobic as shown in Figure 2b. Figure 2c show the transmittance (in red line) of the ambiently-dried aerogel, 90%, that is marginally higher than the best literature transmittance of ambiently-dried aerogels.

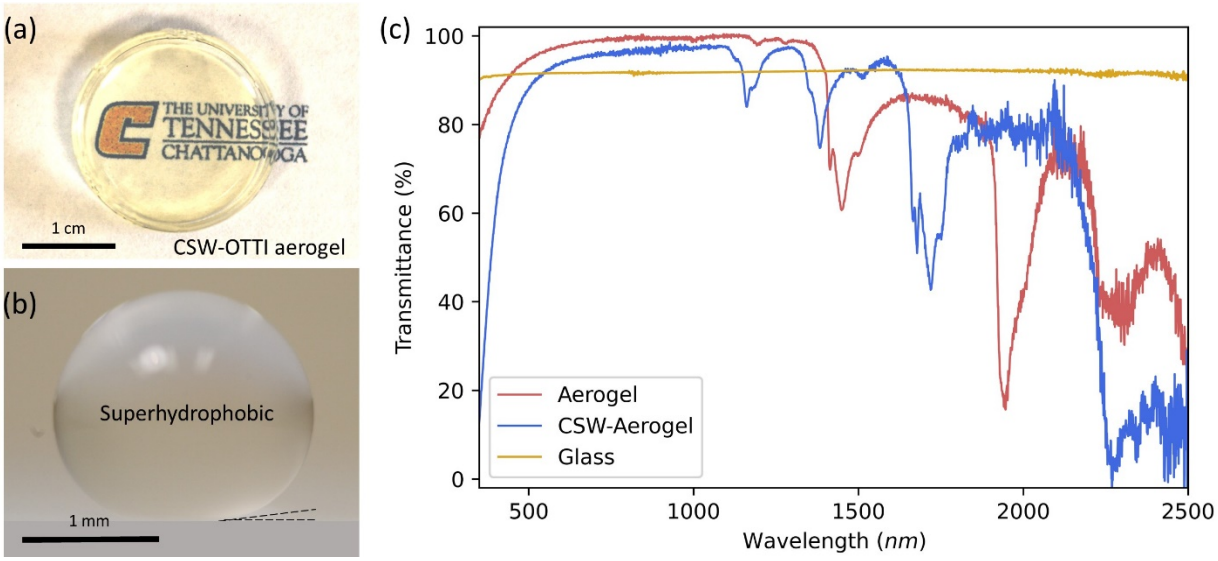


Figure 2: (a) Image of a synthesized CSW-OTTI aerogel. (b) Image of a droplet on a CSW-OTTI aerogel demonstrating its superhydrophobicity with a high contact angle (> 150°) (c) Measured hemispherical transmittance of conventional OTTI aerogel dried by CPD (red), CSW-OTTI aerogel (blue), and glass (yellow). CSW-OTTI aerogels show high transparency in the solar spectrum which is higher than the highest reported in the literature.

2. Optical and thermal modeling via RTE and Mie theory

To perform the proposed thermal modeling solving RTE equation with energy balance equation, specific extinction coefficient of the samples is required. Figure 3a shows transmittance of the samples in IR band by using FTIR. Extinction coefficient as well as specific extinction coefficients are deduced from the FTIR results as shown in Figure 3b and 3c with measured density of the sample. Lastly, the effective emittance of the samples is calculated as shown in Figure 3d. Carbon components in ambiently dried aerogel demonstrated lower effective emittance.

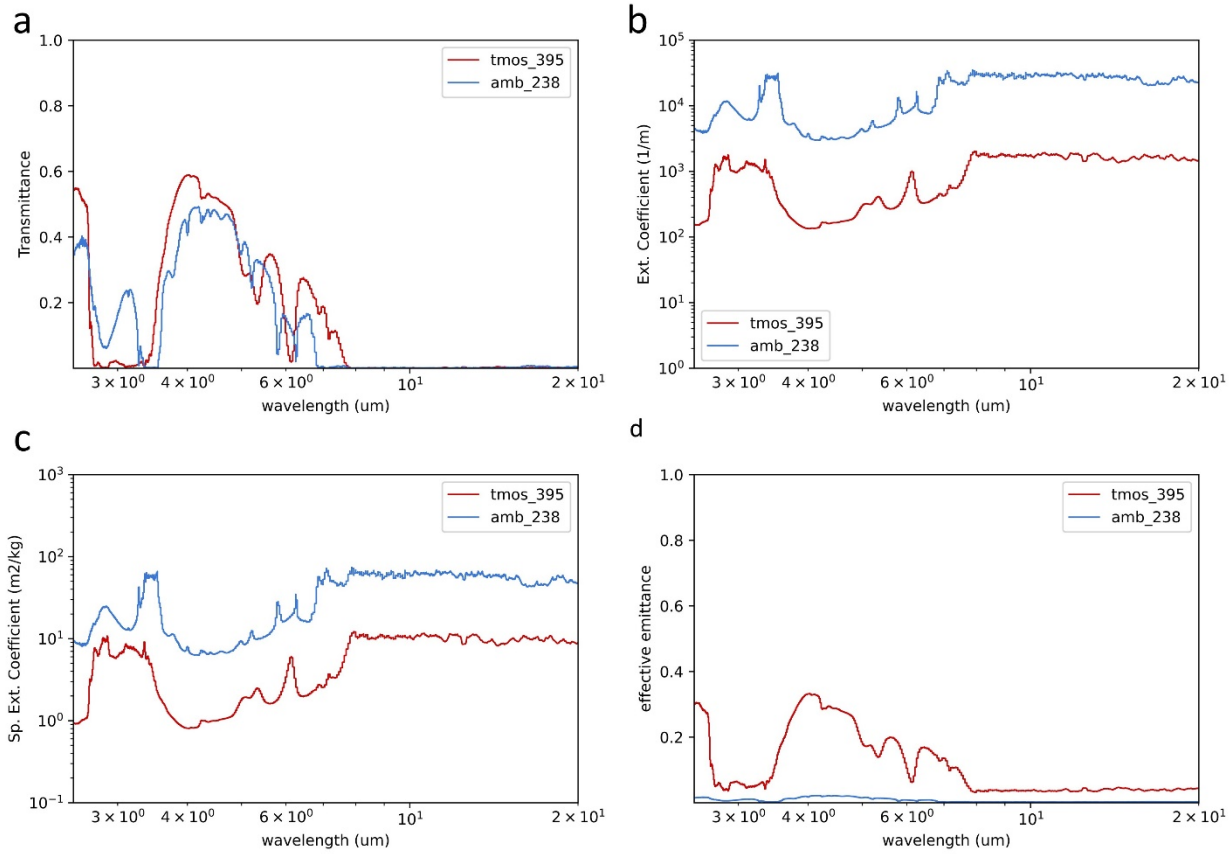


Figure 3: (a) FTIR transmittance of silica aerogel and ambiently-dried aerogel. (b) extinction coefficient and (c) specific extinction coefficient of silica aerogel and ambiently-dried aerogel (d) effective emittance of silica aerogel and ambiently-dried aerogel.

2. Building a lab-scale solar collector

As shown in Figure 4, we have built a lab-scale solar thermal collector, which will be used for outdoor testings.

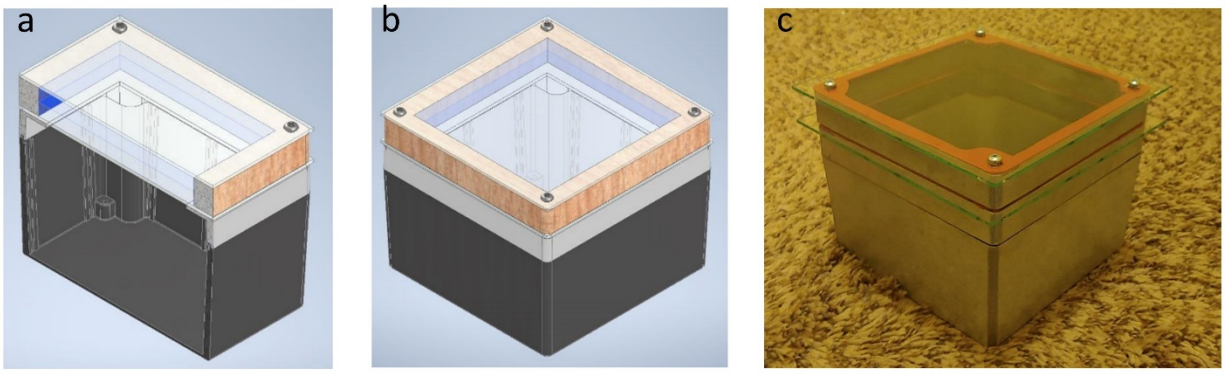


Figure 4: (a) and (b) CAD drawings of solar grill system (c) an image of the built solar grill system before the addition of transparent aerogel

Fiscal Year 2021 Final Project Report

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

Eleni Panagiotou

Co-PI(s): N/A
Other Personnel: Quenisha Baldwin, Akua Maame Korsah

Project Title: A Topological Analysis of Viral Glycoproteins- Application to the Spike Protein of SARS-CoV-2

Date Submitted: 06/20/2020

Award Start – End Date: July 1, 2020 – June 30, 2021

Non-Technical Summary:

A part of the viral life cycle involves viral recognition/binding with the host cell and subsequent fusion/penetration of cell or endosomal membrane (Dimmock 2007, Levine 1992). This research is focused on disrupting the ability of the viral glycoprotein to recognize its receptor or the ability to rearrange its three-dimensional conformation, thereby disrupting the viral life cycle. We propose to use topology to screen for binder molecules to the Spike protein of SARS-Cov-2 and for specific locations of binding along the Spike protein that would disrupt its function. More precisely, we propose to use topology to (1) predict residues of high conformational activity from a 3D structure and (2) to combine chemistry, topology and geometry to quantify the binding affinity of small molecules to the receptor binding domain of glycoproteins.

PROJECT TITLE A Topological Analysis of Viral Glycoproteins- Application to the Spike Protein of SARS-CoV-2

Technology Area of Interest: Advanced Modeling and Simulation

TECHNICAL APPROACH	OUTCOMES
• The local topological analysis of proteins • The local topological analysis of SARS-CoV-2 • DFT simulations and the geometry of binders to the spike protein	The results were submitted for publication at the following journals: • Baldwin, Q. and Panagiotou E., 2021, The local topological free energy of proteins Journal of Theoretical Biology (under minor revision) • Baldwin, Q., Sumpter, B. G. and Panagiotou E., 2021, The local topological free energy of the SARS-CoV-2 spike protein (submitted-under revision) • Panagiotou, E., Vuong, V. Q., Irle, S. and Sumpter, B. G., 2021, Geometry as a screening tool for strong binders to the SARS-CoV-2 Spike protein (submitted) The results were presented at: • Research Dialogues, UTC • Applied Knot Theory Workshop 2020, UTC • AMS Southeastern Fall Sectional meeting 2020, Contributed Session, UTC • BMSE/MCDB joint seminar, UCSB
RESULTS	**OTHER INFO**
	Budget and Schedule Total Budget: $ 19,965 Actual Used: $14,621.80 Balance: $ 5,343.20 Total period of performance is 12 months. **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • 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

Objective 1: Detection of residues of high conformational activities

To predict residues of high conformational activity, we examined the topology of glycoproteins, before and after infusion in the cell. Such crystal structures are obtained for some viruses and are reposited in the Protein Data Bank (PDB). The proposed focused on the following:

Step 1: We created measures of topological complexity particular to proteins.

Step 2: We focused on the following well studied viruses:

- Influenza (PDB files 2HMG and 1HTM)
- Paramyxovirus (PDB files 2B9B and 1ZTM)
- Tick-borne encephalitis (PDB files 1SVB and 1URZ)
- Vesicular stomatitis (PDB files 5I2S and 5I2M).

Our results will provide a topological model for predicting the residue activity of these proteins which we will compare to previous results.

Step 3: We used our model to predict the residue activity of SARS and SARS-Cov-2.

Objective 2: Topological screening of binder molecules

To find binder molecules to the Spike protein of SARS-Cov-2, we used topology as a screening tool. The proposed work will focus on the following:

Step 1: We used DFT calculations to obtain optimized 3-dimensional structures of ligand molecules.

Step 2: We studied the topology/geometry of the obtained ligand conformations to measure their topological compatibility with the Spike protein and suggest ligand molecules.

Step 3: We compared our model of topological compatibility with the binding affinity provided by molecular simulations in previous studies to benchmark our results.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Creation of a new measure of local topology of proteins	Created and submitted for publication Baldwin, Q. and Panagiotou E., 2021, The local topological free energy of proteins Journal of Theoretical Biology (under minor revision)
Topological analysis of SARS-CoV-2 and other viral proteins	Completed and submitted for publication Baldwin, Q., Sumpter, B. G. and Panagiotou E., 2021, The local topological free energy of the SARS-CoV-2 spike protein (submitted-under revision)

	Revisions will be done in the extension of the grant.
DFT simulations and analysis of binder molecules	Completed and submitted for publication Panagiotou, E., Vuong, V. Q., Irle, S. and Sumpter, B. G., 2021, Geometry as a screening tool for strong binders to the SARS-CoV-2 Spike protein (submitted) Anticipated revisions will be done in the extension of this grant.

Challenges & Strategies Used to Address / Overcome:

Time requirements to undertake this research have been substantial and it has been a challenge to teach the students involved and also to conduct the research. Also, it has been challenging to find students capable to contribute to the research. Our strategy was to work very hard.

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

Overall, the proposal worked, but the papers are still under revision. These revisions require substantial effort and time, which is why we need the extension through the next year. I would like to be able to cover a graduate student throughout the year in the proposal, as well as be able to obtain a course release. Especially for such a timely project, I think it is to the benefit of all to advance it fast. Applying for external funding to continue this grant will take place in the next academic year.

IMPACT & OUTCOMES

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

The PI had the chance to advise Quenisha Baldwin, Akua Maame Korsah, Achok Alier and Arielle Beard, all female African American students.

The PI co-authored 3 papers submitted for publication with undergraduate students and with Sumpter B. from ORNL.

These manuscripts have part of the preliminary results required for the PI to apply for external funding:

- Baldwin, Q. and Panagiotou E., 2021, The local topological free energy of proteins Journal of Theoretical Biology (under minor revision)
- Baldwin, Q., Sumpter, B. G. and Panagiotou E., 2021, The local topological free energy of the SARS-CoV-2 spike protein (submitted-under revision)
- Panagiotou, E., Vuong, V. Q., Irle, S. and Sumpter, B. G., 2021, Geometry as a screening tool for strong binders to the SARS-CoV-2 Spike protein (submitted)

Students Impacted

Quenisha Baldwin, a biology undergraduate student from Tuskegee University, submitted for publication 2 papers as first author, gave 3 talks on this work, and visited the group of Carolina Arias at UCSB to do experimental mutations on the Spike protein of SARS-CoV-2 to test our theoretical predictions.

Akua Maame Korsah, UTC, MS Math, proved the asymptotic scaling of the second Vassiliev measure of uniform random walks in confined space.

Arielle Beard (Biology, UTC) and Achok Alier (Chem. Eng., UTC) worked on a related project under URTOPS and presented their results at UTC Research Dialogues.

Community and Broader Impacts

Our understanding of the effects of local topological conformations to the activity of the SARS-CoV-2 Spike protein has the potential to lead to our understanding of mutations and creation of therapeutics. The project was an inter-disciplinary effort to bring together researchers from Mathematics, Biology, and the SimCenter. In addition, participating in this grant gave students valuable experience and education. The students involved were all in minority groups.

The PI gave presentations to students, non-specialists, and multi-disciplinary audiences and published in high impact peer reviewed mathematics and science journals. All the papers were co-authored with undergraduate students (Q. Baldwin and V. Q. Vuong).

Scholarly Products

Publications: All publications were in peer-reviewed scientific journals

1. Baldwin, Q. and Panagiotou E., 2021, The local topological free energy of proteins Journal of Theoretical Biology (under minor revision)
2. Baldwin, Q., Sumpter, B. G. and Panagiotou E., 2021, The local topological free energy of the SARS-CoV-2 spike protein (submitted-under revision)
3. Panagiotou, E., Vuong, V. Q., Irle, S. and Sumpter, B. G., 2021, Geometry as a screening tool for strong binders to the SARS-CoV-2 Spike protein (submitted)

External Conferences:

1. Q. Baldwin, Applied Knot Theory Workshop 2020, UTC
2. Q. Baldwin, AMS Southeastern Fall Sectional meeting 2020, Contributed Session, UTC
3. E. Panagiotou, BMSE/MCDB joint seminar, UCSB

Presentations at UTC:

1. Q. Baldwin, Research Dialogues 2021, UTC,
2. Arielle Beard and Achok Alier, Research Dialogues 2021, UTC

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

This project involved collaborators from ORNL (Sumpter and Irle), students from UTK (Vuong), Tuskegee University (Baldwin), and students from UTC (Korsah, Beard, Alier).

The project involved four undergraduate students from underrepresented groups.

The results were presented in four talks and three papers were submitted for publication in peer-reviewed scientific journals.

EXTERNAL FUNDING

Proposal Submissions

NSF CAREER: Topology of active polymers (recommended for funding)

Contracts/Awards Received

NSF Proposal on Entanglement in Polymers, DMS Computational Mathematics, $125,000.

Sponsored Program Capacity Building Activities

Visited (virtually) NSF to serve as a reviewer.

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 plans to:

1. Complete the publication of the submitted papers
2. Continue this research with new variants of SARS-CoV-2
3. Apply for external funding

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 COVID19. I will pursue research on active matter: entangled polymers with transient crosslinks. Those systems are present in living matter and combine multi-chain entanglement in fluid flows with biopolymer function. I will also pursue to create 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 wish to support students form Mathematics, but have had difficulty in finding them. Another barrier is the teaching load. As my research grows and attracts external funding, it is important to maintain this activity.

FINANCIAL ACCOUNTING

Due to COVID-19, remaining funds for supporting students were carried over.

Fiscal Year 2021 Final Project Report

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

Andrew W. Bailey, Ph.D., Lead PI

Co-PI(s): Gregory Heath, D.H.Sc., M.P.H.; Epidemiology/Public health and preventive medicine expert. Charlie Mix (UTC IGTlab Director); GIS mapping and machine-learning analyst.

Project Title: People, Planet and Profits: Strategic Planning for Outdoor Recreation, Conservation, and Tourism

Date Submitted: July 30, 2021

Award Start – End Date: July 1, 2020 – June 30, 2021

Non-Technical Summary

This project was built upon five interdependent goals, each with individual and cumulative value for the local and scholarly communities. First, estimates of visitation to parks and natural areas in the 16-county region were established using innovative cell phone tracking data combined with manual and auto-trail counters. Visitation growth rates and park size were then utilized to determine carrying capacity and predict future environmental impairment. Next, economic values were then estimated for all protected areas based on tourism impacts from nonlocal visitors, prevention of medical costs due to increased physical activity in outdoor areas, and reduced costs of air and water mitigation procedures due to large tracts of naturally filtering land features. Projected gains and losses of these economic values were also imputed based on rates of development and climate change models. Finally, these data were geospatially analyzed to present a model of highly valuable (i.e., high tourism, high environmental mitigation, and high public health value) and vulnerable tracts of land (i.e,. areas of connected habitats, high levels of biodiversity, and high climate resilience). The final model was produced through an iterative machine-learning process to determine regional assets of high value and vulnerability that support the flourishing of humans, nature, and regional economic benefits.

These outcomes will provide important models for land managers and regional planners as the 16-county region experiences continued development increases in tourism. Collaboration between Chattanooga City planners, Thrive Regional Partnerships, and county, state, and federal land managers were instrumental in the successful completion of this research. Four graduate students and more than 70 undergraduate students were involved in data collection and analyses with three conference presentations already complete. One refereed presentation, delivered by an undergraduate student, was awarded a third-place prize for best conference presentation. Analyses are currently being finalized, and future presentations and publications are forthcoming. Additional lines of research, based on outdoor physical activity

and preventive health during the COVID pandemic, are also being exploited given the timing of project implementation. The data, models, and partnerships leveraged for this research will produce continual success through community collaborations as well as research and grant proposals.

Conservation and Public Health: People, Planet, and Profits: Strategic Planning for Outdoor Recreation, Conservation, and Tourism

TECHNICAL APPROACH	OUTCOMES
Three-year visitation estimates were established using cell phone tracking data. These estimates informed valuation of park spaces through IMPLAN tourism economic impact multipliers, CDC burden of disease indicators, and environmental mitigation data. Combined data were mapped and analyzed with optimal hot spot analyses, a machine learning process that identifies spatially significant clusters of hot and cold spots based on given criteria.	Working partnerships with local, regional, and state entities. Multiple models illustrating the recreational, health, and conservation values of regional green spaces. Three presentations, including one recognized as a top three of the conference proceedings. Multiple presentations, manuscripts, and a grant proposal in progress. New lines of research based on the influence and opportunity afforded by green space during the COVID pandemic. More than 70 students impacted as data collectors, analysts, and presenters of research.
RESULTS	**OTHER INFO**
See Appendices for Tables and Figures.	Budget and Schedule Total Budget: $76,577 Actual Used: $51,681.82 Balance: $24,895.18 Total period of performance is 12 months. Task 1: Staff hired, survey & field data collected, big data sorted, GIS identified. Task 2: Sorting big data & combining data for analyses. Task 3: Merging data geospatially and conducting preliminary analyses. Task 3: Iterative GIS-based analyses for optimal outcome reporting. Deliverables UTC HHP: Andrew-Bailey@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

This project consisted of six interdependent goals that provided a scaffolding for research. The first and most daunting was to estimate visitation to parks and green spaces in the 16 county Thrive Region surrounding Chattanooga. Given the lack of historical record keeping and sparse communication and connectivity across land management agencies, this endeavor required starting from scratch. Multiple methods were initiated, but the final process involved analyses of vast cell phone tracking datasets, combined with geospatial layering to determine visitor origin and county residence. The data was combined with existing information from the IGTLab to create a “carrying capacity” metric based on visits per acre and three-year growth rates in visitation. Carrying capacity is a key indicator of environmental stress and future impairment as a result of overuse. Park size and visitation were then used to estimate economic value to the Thrive Region. Visitors who originated outside the Thrive Region were identified as tourists, and estimates of expenditures were applied to each visitor based on previous research conducted by the UTC Tourism Center and IMPLAN multipliers for each of the 16 counties in the region. These multipliers impute the average annual ripple effect of each dollar spent in the county before the money is leaked outside of the region. Also included in the economic assessment (goal 3) was the preventive health value of park space and prevention of common air and water mitigation procedures for undeveloped land in the region. These values have been established through previous research and are based on increased physical activity of park visitors as well as natural prevention of flooding, water treatment, and air quality issues provided by acres of undeveloped landscapes. These three goals alone provide ample evidence of the true value of green space in the region, supporting local land managers, tourism providers, and recreation conservation advocates in planning and promotion.

Two final models were then imputed using geospatial modeling, machine learning, and hot spot analyses. High value areas were identified as those with high visitation, elevated tourism multipliers, and health benefits as well as high richness of imperiled species and climate resilience. These were combined using a suitability modeling approach and classified into a common scale for illustration. A similar model was created to identify highly vulnerable areas as defined by high carrying capacity, high climate impact, and habitat least cost paths. These two models were then overlaid to produce a final model indicating tracts and corridors with the highest economic, health, tourism, and conservation values which exist in the most vulnerable locations in the region. These models provide valuable guiding information for regional planners seeking to maximize economic values through regional development while maintaining a sustainable ecosystem to support human and environmental thriving.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Goal 1: To establish a baseline and trend of recreation usage in the Thrive Region.	An estimate of visitation to 168 regional locations is presented in Figure 1 based on cell phone data, auto, video, and manual counts (Figures and Tables in Appendices).
Goal 2: To establish a baseline and forecast trends of environmental impacts of recreational use.	Carrying capacity metrics for each monitored site can be seen in Figure 2, overlaid onto 15-year development rates. This is a common indicator of environmental impacts, realized or imminent.
Goal 3a: To estimate economic values of natural areas in the region based on tourism expenditures.	Table 1 provides a summary of economic impacts for each county as estimated through IMPLAN multipliers using average daily expenditures for visits to the region.
Goal 3b: To estimate economic values of natural areas based on preventive health and prevention of environmental mitigation.	Table 2 illustrates the mitigation value of undeveloped land and preventive health values of park space to each county. Figure 3 illustrates the burden of disease by county with a description of park visitation as a preventer.
Goal 4: To forecast the impacts of increased development, increased usage, and climate change on environmental values.	Table 2 illustrates the economic value of undeveloped land to each county and the potential loss to 2060 as imputed by current levels of development and climate models.
Goal 5: To identify high value and highly vulnerable areas based on recreation and tourism impacts, as well as biodiversity and sustainability of habitat cores and corridors.	Figure 4 provides a regional map, displaying areas of high value and vulnerability which should be prioritized for protection to enhance health, recreation and tourism assets, and the regional economy.
Additional findings: Impacts of COVID on visitation to regional parks and green spaces.	Many parks were closed during the COVID pandemic, while others experienced double or triple their average visitation rates. Figure 5 provides an overview of visitation changes from 2019 – 2020 as the pandemic unfolded. These numbers will be compared with COVID infection rates and other health data in the coming months.

Challenges & Strategies Used to Address / Overcome

We were able to achieve the goals as proposed, but our methods had to be modified due to COVID policies and closures. Our original plan was to rely mainly on manual counts of visitation to regional areas with auto-counters and land manager estimates for validation. While students did complete manual counts and identify areas of environmental impact, many were not residing in Chattanooga, were sick or quarantined, and were otherwise unavailable during vital periods of data collection. Instead of relying on student work, we shifted to the analysis of Safegraph cell phone tracking data as our main source of visitation estimation. This required a mental shift as well as many more hours for the PI downloading, organizing, and analyzing huge datasets. It turned out to be a fortunate shift as this method will continue to be a reliable and sustainable data source for the foreseeable future now that the process has been mastered.

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

We were able to meet all goals, but certain methods were less productive than anticipated, mainly due to COVID issues. We had originally hoped to receive visitation and environmental impact information directly from land managers. Unfortunately, many were not in the office during COVID closures, and others just did not respond during the chaos. Our second method of gaining this information was almost as disappointing. Students used a geographic survey app to collect parking lot car counts and document environmental issues on local trails over the course of the semester. Technical issues with the app, combined with difficulties of communicating from a distance during online only classes, rendered much of the data unusable. Finally, constant quarantines and COVID scares made it difficult to schedule student collection times, and both undergraduate students that were hired for the project were prevented from collecting data for a portion of the study. In the end, we were able to achieve the goals through other means, but the take home lesson is to have backup plans for your backup plans and to remain flexible in crazy times.

IMPACT & OUTCOMES

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

The biggest career impact will be future collaborations and future projects generated by this research team. This successful cross-departmental collaboration has demonstrated the utility of combining tourism, conservation, and health metrics to advocate for sustainable development in the region. That message resonates well with city and county planners as well as local non-profits supporting rural development around local municipalities. The combined use of big data (Safegraph), geospatial analytics, and machine learning techniques positions UTC well for future projects requiring advanced modeling and forecasting. The outcomes of this research also enable us to proffer a positive message about the value of conservation and recreation. Given the tendency for messengers of sustainability to sound like doomsayers, the health and

economic benefits of outdoor recreation provide an alternative hopeful approach to conservation initiatives. This combination of new analytic techniques (big data mining, geospatial machine learning) and the joining of novel datasets, creates an opportunity for many collaborative projects in the future, as well as the solicitation of support through grants and foundations.

Students Impacted

Sarah Kelehear (M.S. candidate-Environmental Science, Summer 2021): Sarah was involved in survey development and deployment, land manager communication, visitation estimation, GIS data acquisition and preparation, and field-based data collection. She was also the point person in identifying the Safegraph dataset and filtering the data for preliminary analyses. Sarah acquired full-time employment and exited the project in January 2021.

Jeremy Page (M.S. candidate- Athletic Training, Summer 2021): Jeremy helped with survey data collection and field-based data collection for visitation and documentation of environmental issues. He was a main contact for local land managers and did a lot of data management for the Safegraph visitation data once it was in spreadsheets.

Brandon Denney (M.S. candidate- Public Health, Summer 2021): Brandon handled the data acquisition and preparation for health and economic impacts for the 16 county region.

Alayna Smith (B.S. SORT mgmt, May 2021): Alayna aided with visitation estimates, and field-based data collection of environmental issues on regional trails. Alayna presented visitation data from this project at the Southeastern Environment and Recreation Research (SERR) conference in March 2021. She was awarded the 3rd place overall prize for best undergraduate presentation.

Isaac Talbot (B.S. SORT mgmt, May 2021): Isaac also aided with park visitation and field-based data collection. COVID issues limited his availability for much of the project.

Outdoor Recreation class (HHP 3060): This online course has involved 66 students in field-based data collections using the GIS collector app for iPhone and Android. Students documented 3 environmental issues on local trails to help establish a baseline from which to measure change over the next decade. They also collected information at trailheads regarding visitation, recreation user types, and tourism (i.e., license plate info). This process was valuable for them as they were taught various methods of visitor estimation and were introduced to GIS software utilized by all recreation & conservation land managers.

Community and Broader Impacts

Perhaps the most salient impact of this project is to summarize and illustrate the true value of protected green spaces in the Thrive Region. Valuation of open space is inherently messy, and the terminology is often abstract. Creating models that account for recreation, conservation, tourism, and health values of our region will ensure that this information is part of the conversation for regional planning and development. Without the appropriate language to express the value of our outdoor treasures, planning agencies may neglect them and Chattanooga could unintentionally degrade a key aspect of our identity. Conversations have

already begun with the Thrive Regional partnership, Chattanooga Smart City data managers, and state, county, and city land managers regarding intelligent planning and use of natural resources. The charts, models, and maps produced through this collaborative project will serve as a foundation for sustainable planning.

Publications and presentations will also broaden the message and generate ideas for new directions. This research has already piqued the attention of researchers (See SERR research award below) and City managers, who are interested in utilizing similar data in their research. When these results are shared more widely, we anticipate a similar response as we push the limits of scientific inquiry in the recreation and tourism disciplines.

Scholarly Products

Publications:

1. Forthcoming

External Conferences:

1. Bailey, A. & Smith, A. (2021). Of parks and pandemics: Visitation disparities across county lines. Presentation for the Southeastern Recreation Research Conference (virtual, refereed); March, 2021

Presentations at UTC:

1. Bailey, A. & Smith, A. (2021). Of parks and pandemics: Visitation disparities across county lines. Presentation for UTC Research Dialogues (virtual); March, 2021
2. Bailey, A., Heath, G.W., & Mix, Charlie (2021). People, Planet, & Profits: Strategic planning for outdoor recreation, tourism, and conservation (virtual). A CEACSE presentation for UTC Research Dialogues; March, 2021

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

Thrive Regional Partnership will be a big beneficiary of the outcomes from this project, and they will be an ongoing partner. Matt Reed is the main contact for the Natural Treasures division and we will be discussing ongoing research opportunities when we present our final report to them.

The Trust for Public Land has been a continual partner in parks research, especially as it pertains to public health. David Johnson is attentive and responsive to all grant and research opportunities we have discussed.

Local non-profits are ambitious partners for research and grant proposals. Informal discussions initiated from this project have included Lula Lake, SORBA Chattanooga, Southeastern Climbers Coalition, Land Trust for TN, TN River Gorge Trust, Southeastern Conservation Corps, and WaterWays.

Finally, regional governments and tourism agencies have shown interest in this project: Southeast TN Tourism Association, City of Chattanooga, Hamilton County Parks & Recreation, and various municipal authorities associated with the Thrive Regional Partnership (Dunlap, TN; Jasper, TN; Dalton, TN, etc.).

EXTERNAL FUNDING

Proposal Submissions

None have been submitted, yet, but discussions have begun with members of the Thrive Regional Partnership and the Trust for Public Land. Specifically, a park planning grant through the Robert Wood Johnson Foundation or a similar opportunity through the Department of the Interior is being explored.

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?

This project has solidified collaborative partnerships between UTC and community organizations that will continue to bear fruit. Outdoor recreation and conservation metrics are becoming vital for planning agencies, and visitation, economic impact, and health impact data are central to their initiatives. Continued assessment of visitation, environmental, and economic impacts will strengthen relationships with land managers (state & local), regional planning agencies (Thrive, TPL, RPA), tourism agencies (SETA), and program providers (Outdoor Chattanooga, Hamilton County Parks & Recreation).

We also plan to explore health-related data in a deeper way once we have pursued publications and grants based on our original project goals. The availability of health and visitation data at the census tract level provides the opportunity for granular level insights that were not previously attainable. Additionally, the preparation of data over the course of the COVID pandemic provides a secondary research agenda that was not anticipated in the original project proposal. Understanding the true influence of outdoor recreation and park accessibility on mental and physical health is a priority in environmental research at present, and the data collected over the course of this project provides us with a unique advantage relevant to that line of research.

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

We will continue conducting research on visitation and economic impacts now bolstered by methods learned through our CEACSE project. We have a project scheduled with the Southern Off-Road Bicycling Association (SORBA) next year to assess economic impacts of mountain biking in the region. Prentice Cooper State Park has expressed strong interest in the creation of a recreation plan based on visitation and user profiles. Thrive Regional Partnership and the Trust for Public Land will also provide ongoing research opportunities in an effort to paint a picture of regional influence of recreation and conservation on economic and public health.

Research on the physical and mental benefits of outdoor activity will also persist. Currently, a project for Fall of 2021 is being finalized to measure the mental impacts of outdoor education programming in public schools. This is possible through a partnership with WaterWays, a local non-profit providing public school programming at Enterprise South Nature Center. Dr. Bailey has joined an advisory board for the Hamilton County Department of Education, which will likely lead to additional research in that line.

A key finding that has emerged from this multi-disciplinary effort is that visits and access to parks, trails, greenways, and public spaces result in a greater probability that visitors will actually engage in meaningful levels of physical activity that may result in improved health and reduced costs due to chronic conditions or diseases. However, the current scientific literature begs the question as to whether or not such visits actually impact a persons' total physical activity. Therefore, an important extension of the present work will be to identify a cohort of representative people who visit our regional parks, trails, and greenways and follow them prospectively with objective measures of physical activity to assess the impact on total physical activity, health status, and disease 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?

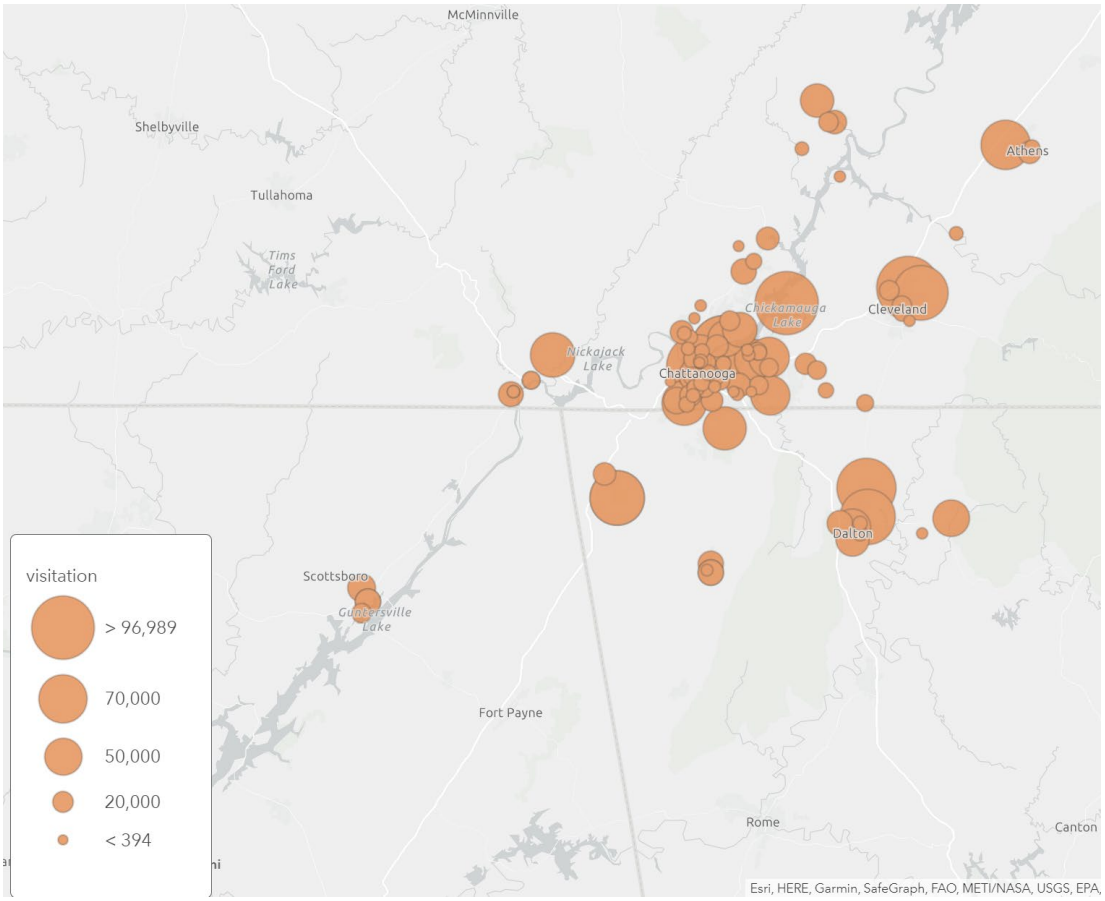
Our main barriers will be human resources as projects continue to develop and evolve. There are only a few researchers at UTC pursuing similar lines of research and few graduate programs directly associated with the topic. The public health program is now officially up and running, so that will provide an ongoing opportunity for student resources. Undergraduate students provide some support, though their capacity for leadership is limited by lack of experience. Grants may provide teaching releases for PIs which could create space for more research productivity.

FINANCIAL ACCOUNTING

We had a substantial amount of funding left unused, mainly due to the lack of student availability during the pandemic. We had budgeted for two undergraduate and graduate students for the entirety of the project, but it became extremely difficult and inefficient to rely on student aid with extended quarantines and major life transitions during difficult times. Most of the unused funds reflect this lack of student research pay. As a result, we shifted our method of visitation assessment to the use of big data via Safegraph cell phone tracking. Originally, we re-budgeted for the purchase of this data but soon discovered that it is much more affordable for educational researchers. Thus, direct costs were much less than anticipated, but there was a much steeper learning curve for the PI. In the end, all goals were met, so the project was a success.

Appendices

Figure 1. Comparison of visitation at regional green spaces (2019).



Utilizing Safegraph® cell phone tracking data, we established a baseline and trajectory of visitation to natural spaces in the area.

- Visitation increased 15% or more from 2018-2020, with larger increases in 2020 due to the COVID-19 pandemic.
    - 30% of visitors originated outside the Thrive region, indicating a significant tourism potential
        - Increased visitation has not been supported by equivalent increases in funding.
        - High visitation areas include river-adjacent areas in Hamilton County, and State Parks throughout the region.

Figure 2. Loss of undeveloped land (hot spots) and carrying capacities of regional parks.

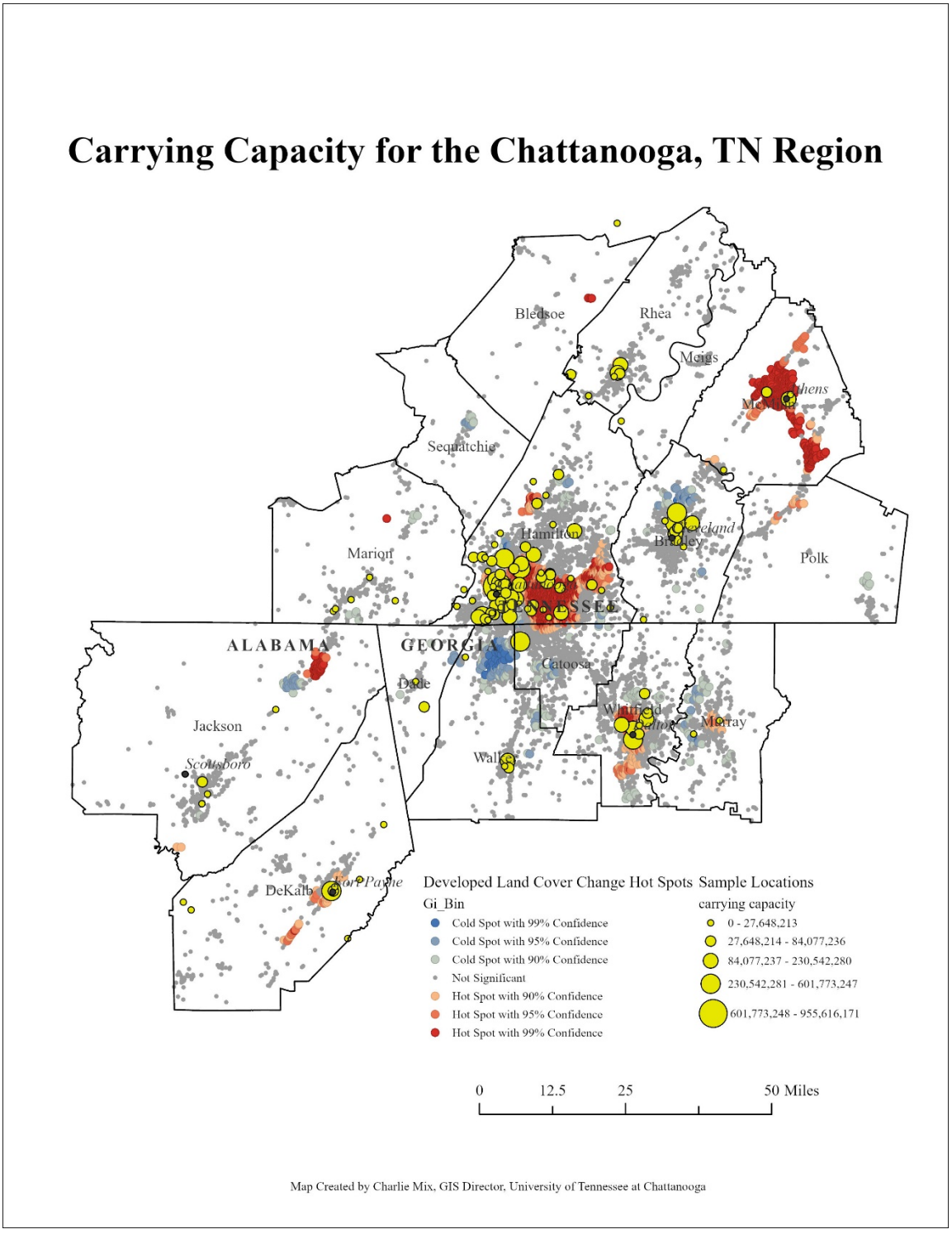


Table 1. Economic impacts of parks based on visitation and average daily expenditures.

County	Multiplier	Daily Total Impact	2019 visitation (Sample)	Total Impact	State Taxes	Fed Taxes
Bledsoe	1.218978102	334	28250	$9,435,333	$762,737	$649,739
Bradley	1.442675159	453	576086	$260,966,732	$21,315,164	$20,162,993
Catoosa	1.365930599	433	90288	$39,094,704	$2,979,504	$2,437,776
Dade	1.223974763	388	151115	$58,632,426	$4,080,092	$4,080,092
DeKalb	1.441269841	454	116181	$52,746,174	$3,833,973	$3,136,887
Hamilton	1.662420382	522	2731488	$1,425,836,736	$98,333,568	$109,259,520
Jackson	1.331230284	422	191409	$80,774,598	$6,125,088	$5,359,452
Marion	1.302547771	409	138501	$56,646,909	$4,986,036	$4,432,032
McMinn	1.337579618	420	164466	$69,075,720	$6,249,708	$5,098,446
Meigs	1.206030151	240	4001	$960,120	$68,009	$72,009
Murray	1.217665615	386	74391	$28,714,926	$2,082,948	$1,934,166
Rhea	1.257961783	395	303132	$119,737,140	$11,215,884	$7,881,432
Walker	1.203225806	373	85016	$31,710,782	$2,890,527	$1,870,341
Whitfield	1.391167192	441	560801	$247,313,021	$16,263,215	$15,702,414
Total	1.514515745	474.5289	5215122	2474726240	181451765.5	181236264.5

The Chattanooga region is renown as an outdoor destination, bringing in tourists from all over the world.

- Tourism dollars support local economies, and multiply with continued local expenditures.
    - The average outdoor tourist to the region spends $315/day, injecting money directly into the economy. The total impact varies by county industry and visitation.
    - Tourism impact factors, combined with visitation and percent of protected acres in each county, account for 12% of variance in physical inactivity and self-reported poor health. Outdoor recreation promotes local activity as well as tourism.

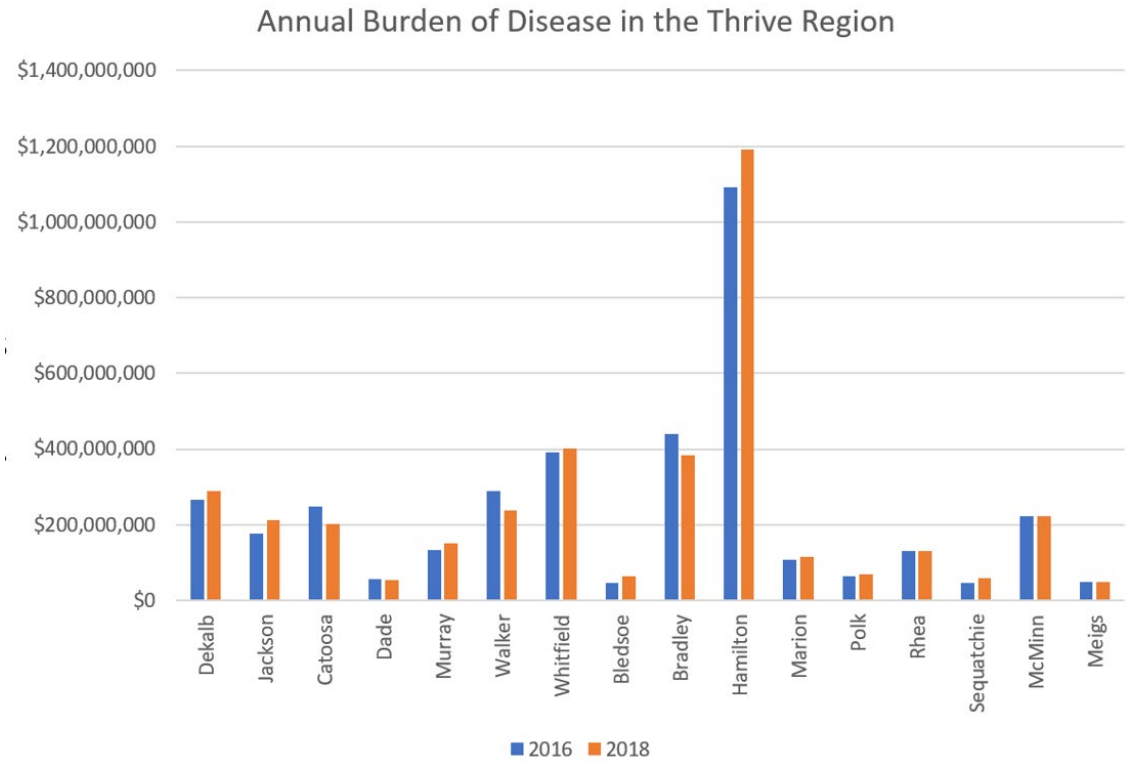
Table 2. Tourism, environmental mitigation, and health values of green space with annual projected losses in 2060.

County	Tourism Revenue	Air Mitigation	Water Mitigation	Health Values (Park Space)	%15yr Development	Total CC Visit Loss	Annual Tourism Loss to CC (2060)	Annual Mitigation Loss (2060)
Bledsoe	$9,435,333	$15,767,694.38	$124,219,394.82	$6,616,945.87	0.02	-13682	-$764,561.11	-$5,169,140.08
Bradley	$260,966,732	$14,855,701.23	$117,034,626.15	$925,858.17	0.10	-245865	-$13,531,607.94	-$26,334,857.86
Catoosa	$39,094,704	$6,332,498.86	$49,888,027.82	$2,266,733.42	0.18	-42690	-$1,357,429.48	-$20,134,699.04
Dade	$58,632,426	$5,369,713.38	$42,303,112.36	$2,359,210.18	0.03	-353702	-$47,175,785.49	-$2,839,166.21
DeKalb	$52,746,174	$37,922,335.15	$298,755,760.37	$4,234,914.84	0.03	-52642	-$10,896,555.93	-$23,436,235.88
Hamilton	$1,425,836,736	$19,280,707.32	$151,895,244.65	$11,943,055.02	0.11	-1422406	-$110,009,170.32	-$36,703,857.95
Jackson	$80,774,598	$39,967,128.07	$314,864,833.34	$22,154,282.50	0.05	-108972	-$10,157,808.77	-$35,669,222.20
Marion	$56,646,909	$10,127,593.90	$79,786,147.27	$15,194,832.34	0.06	-77704	-$6,848,072.32	-$11,406,508.09
McMinn	$69,075,720	$20,741,685.42	$163,404,968.96	$1,844,678.53	0.05	-96774	-$5,808,768.33	-$18,468,909.82
Meigs	$960,120	$9,812,037.34	$77,300,162.66	$3,120,064.30	0.02	-2001	-$164,156.91	-$4,060,396.91
Murray	$28,714,926	$12,107,594.42	$95,384,779.48	$21,819,607.36	0.06	-179469	-$21,545,490.89	-$13,597,277.60
Rhea	$119,737,140	$13,714,966.80	$108,047,811.86	$5,805,032.01	0.07	-149117	-$12,022,824.57	-$17,265,143.25
Walker	$31,710,782	$16,541,230.11	$130,313,382.82	$20,025,118.58	0.07	-59389	-$2,988,052.86	-$19,435,417.82
Whitfield	$247,313,021	$11,863,448.60	$93,461,375.51	$5,009,328.11	0.07	-266359	-$13,808,690.05	-$15,115,718.20
Total	**$2,474,726,240**	**$19,272,419.61**	**$151,829,953.31**	**$10,363,692.94**	**0.09**	**-3070777**	**-$259,332,840.81**	**-$30,340,024.46**

If current trajectories in land development continue, losses in environmental mitigation (air and water contamination) will be more than $30 million annually for the region.

Climate change models predict a 6% decrease in active recreation for the Southeastern U.S. by 2060, mainly due to hotter summers with no real shoulder seasons and increased precipitation volumes and flooding. Adjusted for type of recreation use in the Thrive Region, this would equal almost $260 million in tourism losses annually.

Figure 3.



The Thrive Region is a health poor hotspot. This lower quality of life inflicts an additional burden of economic disparities due to medical expenses and loss of work.

- The chart above illustrates the direct and indirect (i.e., loss of work) costs of five major preventable illnesses (heart disease, breast and colon cancer, stroke, and diabetes).
- Physical inactivity and lack of access to activity sites predict up to 35% of the variance in these combined conditions in the Thrive Region.
- Physical inactivity was also significantly correlated with the health outcomes of type 2 diabetes, colon cancer, breast cancer in women, coronary heart disease, stroke, and poor mental health. Hence, explaining in part the significant amount of variance in the model contributed by physical inactivity. These findings have been previously confirmed by Lee et al. 2012.
- In addition, the prevalence of physical inactivity was also significantly associated with deaths from COVID and the COVID case fatality rate across the Thrive 55 Region.
- 70% of visits to protected areas are by local residents, demonstrating their value for illness prevention.

Figure 4. High value and highly vulnerable land tracts in the thrive region.

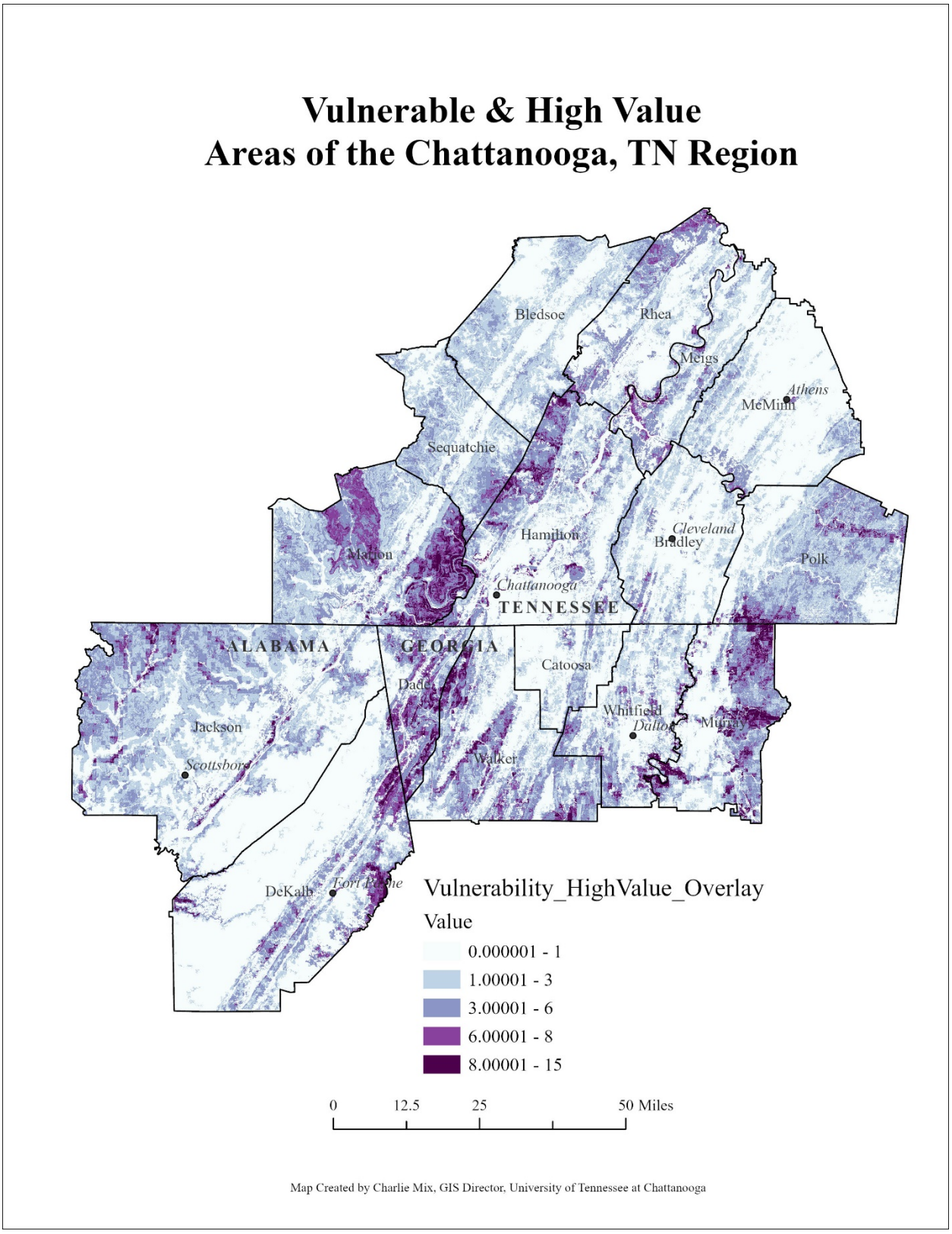
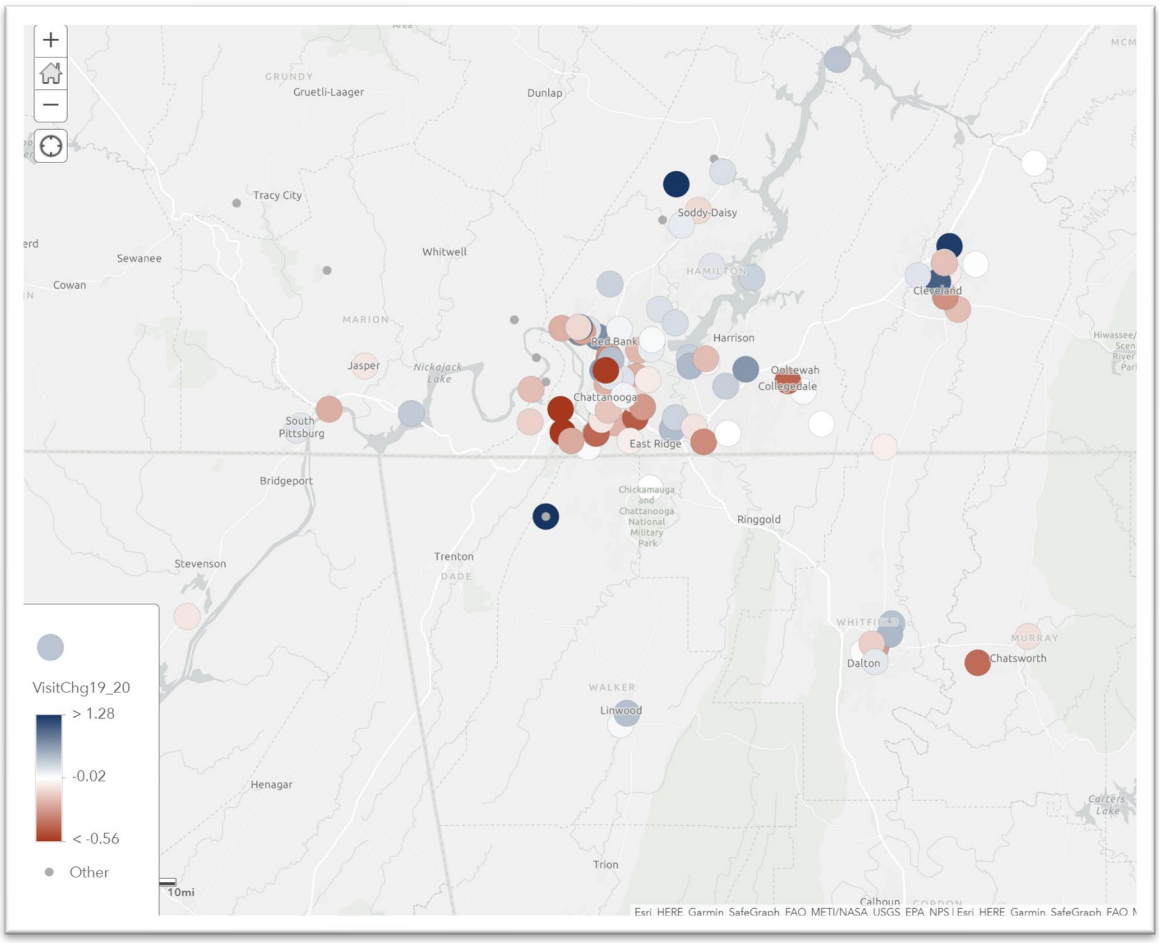


Figure 5. Visitation changes (1= 100%) from 2019 – 2020, because of the COVID-19 pandemic.



Visitation to parks in the region showed disparate trends as a result to nonuniform responses to the COVID pandemic in 2020. Some municipal parks closed for months while county parks remained open, resulting in over-burdening of rural park systems. Visitors stayed longer in the parks but did not travel as far from home. Future analyses will determine the relationship of COVID cases to nonlocal visits in the region.

Recently, a series of systematic reviews examining the impact of parks, trails, and greenways were conducted by Hunter et al. 2019 and the Task Force on Community Preventive Services (2020 – 2021) and indicated that among visitors to parks, public lands, trails, and greenways where an array of physical activity promotion efforts existed (e.g., programming, trail and facility signage, and wayfinding maps) they were 17% more likely to engage in meaningful levels of physical activity. Also of significance within these reviews were the presence of a park, trail, greenway, and public space infrastructure increased visitation by 32%. Hence, park, trail, and greenway infrastructure alone are enough to draw visitors. The authors have suggested that with increased ‘marketing’ and promotion of such spaces, along with physical activity and recreational programming, a greater proportion of visitors can be expected who approach meeting the health and fitness benefits of physical activity.

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Fiscal Year 2021 Final Project Report

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

Reetesh Ranjan, Lead PI

Co-PI(s): N/A

Other Personnel: N/A

Project Title: An Efficient Framework for Numerical Investigation of Turbulent Combustion Using Detailed Finite-Rate Chemistry

Date Submitted: 7/30/2021

Award Start – End Date: July 1, 2020 – June 30, 2021

Non-Technical Summary:

Combustion devices such as liquid-fueled propulsion and gas turbine systems operating under lean conditions are desirable due to their low emission characteristics. Accurate prediction of complex physical processes observed in these devices such as ignition, extinction, pollutant emissions, combustion instability, etc., over a wide range of operating conditions requires the use of detailed finite-rate chemistry. Although recent computational advancements have enabled the use of detailed finite-rate chemistry while performing direct numerical simulation (DNS) and large eddy simulation (LES) of such systems, the computational expense still tends to be huge, thus requiring further strategies for efficient computation. The research carried out under this effort focused on establishing and assessing novel computationally efficient approaches to perform high-fidelity simulations of turbulent combustion using detailed finite-rate chemistry. The first approach focused on implementing and evaluating the hybrid transported-tabulated chemistry (HTTC) technique, where the computational efficiency is attained by reducing the total number of transport equations. The second approach focused on relying on the use of the intrusive and non-intrusive reduced-order modeling (ROM) techniques. Both these approaches have been assessed by simulating turbulent premixed flames at different operating conditions and yielded accurate results in comparison to the reference results in an efficient manner. Additionally, high-fidelity DNS studies have been performed to examine aspects of turbulence-chemistry interactions prevalent in turbulent premixed and non-premixed flames. Specifically, turbulent premixed flames are simulated at elevated pressure and by employing chemical mechanisms with increasing levels of complexity to examine the effects of pressure on the features of flame-turbulence interactions. Furthermore, a canonical non-premixed flame configuration has been simulated to examine the extinction and re-ignition phenomena. Finally, results from the simulation of thermo-acoustics instabilities are examined to characterize the behavior of flame dynamics during such instabilities.

The research effort during the period of performance has resulted in 1 MS thesis, 1 MS independent study, 2 international conference presentations, 2 international conference articles, 4 internal conference presentations, and 2 journal articles that are currently being prepared. The project has also trained 2 graduate students and 1 undergraduate student on simulation, modeling, and analysis of turbulent combustion by using high-performance computing (HPC) resources at UTC. The project has demonstrated the use of HPC resources facilitated by the SimCenter at UTC. So far, under the project, one white paper and two proposals have already been submitted to external agencies and further white papers and proposals will be submitted in the following year.

An Efficient Framework for Numerical Investigation of Turbulent Combustion using Detailed Finite-Rate Chemistry

Technology Area of Interest: Aerospace, Defense, and Energy Applications

TECHNICAL APPROACH

- Establish finite-rate chemistry-based strategy for simulation of turbulent combustion using high-performance computing (HPC) tools
- Implement HTTC and ROM techniques
- Implement subgrid models for LES
- Perform DNS and LES of turbulent premixed flames at elevated pressure and turbulent non-premixed jet flame to examine extinction and reignition
- Develop tools for statistical and spectral analysis of turbulent premixed flames
- Establish UTCFoam (an extended version of OpenFoam) for combustion simulations
- Analyze thermo-acoustics combustion instabilities

OUTCOMES

- Established tools and models for simulation of turbulent combustion in canonical and applied configurations
- Trained 2 graduate students and 1 undergraduate student on simulation of turbulent combustion using HPC tools and analysis of results using Python, Tecplot, and Paraview
- Resulted into 1 MS thesis, 2 international conference articles, 2 international conference presentations, 4 internal conference presentations, 2 journal articles under preparation, and 3 white papers/proposals

RESULTS

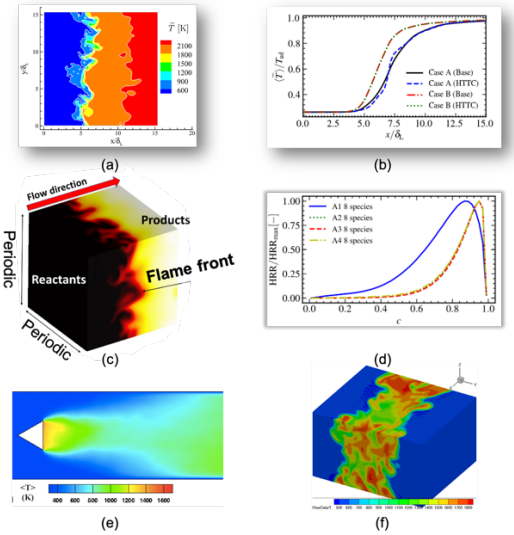

Figure 1 comparison of results from HTTC (solid contours) with baseline (colored contours) in a turbulent premixed flame (a), comparison of HTTC and baseline results for two operating conditions (b), turbulent-premixed flame structure at elevated pressure (c), effect of pressure and operating conditions on heat-release rate (d), temperature from simulation of VOLVO rig (e), and simulation of extinction and reignition in turbulent non-premixed flame (f).

OTHER INFO

Budget and Schedule

Total Budget:	$76,099.00
Actual Used:	$67977.91
Balance:	$8121.09

Total period of performance is 12 months with multiple tasks spread out during the entire year.

Deliverables

- Quarterly report describing numerical methods, techniques, and results that were developed or improved.
- Final report detailing results, financials, and future work
- Publications
- External and internal conference presentations

Organization Information

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ACCOMPLISHMENTS & OUTCOMES

Project Overview

Combustion devices such as liquid-fueled propulsion and gas turbine systems operating under lean conditions are desirable due to their low emissions, compact geometry, and improved efficiency characteristics. Accurate prediction of complex physical phenomena observed in these devices such as mixing, ignition, extinction, emissions, combustion instability, different modes of combustion, etc., over a wide range of operating conditions requires the use of detailed finite-rate chemistry. Large eddy simulation (LES) of such devices is considered to be a promising method as it can capture the unsteady features of turbulent combustion occurring within these systems. Although recent computational advancements have enabled the use of detailed finite-rate chemistry while performing LES, however, the computational expense still tends to be huge, thus requiring alternate strategies. The research conducted under this effort focused on establishing computationally efficient techniques for the investigation of turbulent combustion using detailed finite-rate chemistry. First, the baseline reacting flow solver, referred to as AVF-LESLIE, is improved to enable the use of arbitrarily complex chemical mechanism. Afterward, subgrid models were implemented within the solver to allow performing LES. The finite-rate chemistry-based solver is then extended to include the established hybrid transported-tabulated chemistry (HTTC) approach and the intrusive and non-intrusive proper orthogonal decomposition (POD) based reduced-order modeling (ROM) techniques for efficient simulation of turbulent combustion. The HTTC strategy enhances the computational efficiency by reducing the total number of the transported equations by using self-similar profiles for the minor species and only transporting the major species. The strategy has shown significant computational cost reduction. The POD based intrusive ROM utilizes a Galerkin projection approach to perform model reduction, while the non-intrusive ROM is based on radial basis functions-based interpolation leveraging the pre-computed POD modes to perform the model reduction. All the techniques have been verified comprehensively by simulating freely propagating methane/air turbulent premixed flame at different operating conditions.

The reacting flow solver AVF-LESLIE has also been used to investigate fundamental aspects of turbulence-chemistry interactions in premixed and non-premixed configurations. Specifically, the turbulent premixed flames have been simulated at elevated pressure to examine the statistical, structural, and spectral characteristics of flame-turbulence interactions. The focus of study of non-premixed flame configuration was to verify a setup that has been investigated in the past with the solver considered in this project. In addition, results from the simulation of thermo-acoustics instabilities within the CVRC combustor rig has been analyzed to understand the role of finite-rate chemistry on the flame dynamics. Finally, for the application purposes, some preliminary investigation of the VOLVO combustor rig was performed using the UTCFOAM solver, which is an in-house and extended version of the OpenFOAM software.

The activities carried out under this project have resulted into computational tools, modeling capabilities, and analysis tools, which can be used to examine turbulent combustion characteristics in fundamental and applied configurations. These activities have demonstrated the capabilities within the research group of the PI to carry out fundamental and applied research in the broader area of simulation and modeling of turbulent combustion. The project has also broadened the capabilities of SimCenter at UTC in conducting simulation based investigations of relevance to aerospace, defense, and energy applications. The project has trained both graduate and undergraduate students in the use of HPC tools to solve fundamental and applied problems pertaining to energy conversion and propulsion devices. The project accomplishments in form of computational capabilities, publications, and presentations will allow the PI to work on proposals seeking external funding.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Extend reacting flow solver for handling of different types of chemical mechanism	Added the Cantera interface and improved the existing Chemkin interface to handle arbitrarily complex chemical mechanisms
Establish HTTC and ROM strategies for turbulent combustion	Implemented the HTTC and ROM strategies in the flow solver
Demonstrate capabilities of novel efficient framework	Assessed capabilities of the HTTC strategy by performing simulation of turbulent premixed flame and comparing with baseline strategy
Examine turbulence-chemistry interaction at high pressure	Simulated and analyzed 8 DNS datasets using two different chemical mechanism and 4 different operating conditions to assess the effects of pressure and the role of turbulent conditions on flame-turbulence interactions
Analyze extinction/reignition events in a turbulent non-premixed flame	Evaluated the solver for its ability to simulate a canonical test case exhibiting extinction and reignition events in a non-premixed flame
Evaluate UTCFOAM for simulation of turbulent combustion	Simulated the non-reacting and reacting flow within the VOLVO rig
Analyze thermo-acoustics combustion instabilities	Data from simulations of the CVRC rig using detailed chemistry has been used to understand flame dynamics during self-sustained combustion instabilities.

Challenges & Strategies Used to Address / Overcome:

A major challenge was related to working with students who had limited or no experience with the use of computational tools. However, a hands-on training experience, collaborative working environment, and weekly reporting from students helped me to address this challenge.

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

Initially, I had the expectations that the graduate students would be able to contribute to some of the code development activities. However, a lack of experience made it challenging, thus leading me to take over the task of the key code development tasks.

IMPACT & OUTCOMES

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

The research work carried out under this effort will have impacts at various levels on the career of the PI in the area of modeling and investigation of turbulent combustion. It has allowed establishing a computational framework, which can be used to carry out fundamental and applied investigation of turbulent combustion, which is observed in energy conversion and propulsion devices. The computational strategy demonstrated under this research has established accurate and efficient approaches for simulation of turbulent combustion while employing an arbitrarily complex finite-rate chemistry based approach, which is key for the prediction of unsteady flame-turbulence interactions under different operating conditions, ignition, extinction, etc. It has further extended the collaborative research work with the researchers from Georgia Tech and Purdue. Furthermore, the high-fidelity simulations conducted during this project have demonstrated the HPC-based modeling and simulation capabilities with the PI's research group. Overall, the resulting computational capabilities, publications, and presentations are helpful to the PI in seeking extramural funding.

Students Impacted

1. **Jamie Bowers** (MS with thesis option, Summer 2021)**:** Ms. Bowers learned carrying out high-fidelity turbulent combustion simulation using HPC resources. Additionally, she learned the skills to analyze large-scale datasets generated from simulations using Python. A key focus was to analyze statistical, structural, and spectral aspects of flame turbulence interactions prevalent in premixed flames. She has been trained on usage of tools such as AVF-LESLIE solver, Tecplot, Paraview, Python, GitHub, Latex, Trac, and Cantera.

2. **Jash Doshi** (MS with non-thesis option, Spring 2021)**:** Mr. Doshi was trained to carry out high-fidelity turbulent combustion simulation using HPC resources. He finished an independent study project focused on examining extinction and reignition occurring within a canonical non-premixed flame. He has been trained on usage of tools such as AVF-LESLIE solver, Tecplot, Paraview, Python, Trac, and Cantera.

3. **Eli Durant** (Undergraduate, expected graduation Fall 2021)**:** Mr. Durant has learned several skills ranging from pre- to post-processing and running the simulations using HPC resources provided by SimCenter. He has learned tools such as Python, Cantera, UTCFOAM, Tecplot, Paraview, Pointwise, Trac, etc.

Community and Broader Impacts

The research carried out during the period of performance addresses challenges associated with turbulent combustion, which is of great importance to aerospace, defense, and energy conversion applications. The activities carried out under this effort will have broader impacts at various levels. The proposed work has extended the expertise of the PI in the area of development of methods and models for the investigation of turbulent combustion. The demonstration of the computational framework has enabled techniques such as HTTC for LES and intrusive and non-intrusive ROM for LES of combustion, which will be accessible to a community of researchers and can potentially

lead to collaborative research activities in the future. For example, it has led to a journal article under preparation collaboratively with the researchers from Georgia Tech and Purdue. The PI has also worked closely with students at UTC, which has prepared them for solving challenging problems associated with combustion devices by using advanced computational tools. The research work leveraged advanced HPC resources facilitated by the SimCenter at UTC, which will extend the current computational capabilities offered by the SimCenter to the external agencies. Finally, the resulting computational capabilities, archival publications, and conference presentations out of this effort will help in seeking external funding.

Scholarly Products

Software:

1. AVF-LESLIE: A fully compressible multi-species reacting flow solver

2. UTCFOAM: In-house and extended version of OpenFOAM

Publications:

1. J. Bowers, E. Durant, and R. Ranjan, “Application of Intrusive and Non-Intrusive Reduced Order Modeling Techniques for Simulation of Turbulent Premixed Flames”, AIAA-2021-3634.

2. V. Hasti and R. Ranjan, “Analysis of Flame Structure During Longitudinal Combustion Instability within a High-Pressure Shear Coaxial Single Element Combustor”, Accepted for Symposium on Thermoacoustics in Combustion: Industry meets Academia (SoTiC 2021), 2021.

3. J. Bowers, E. Durant, and R. Ranjan, “On the Effects of Variation of Pressure, and Length- and Velocity-Scale Ratios on the Features of Methane/Air Turbulent Premixed Flames”, Under Preparation, 2021.

4. A. Panchal, S. Karpe, R. Ranjan, and S. Menon, “Application of Hybrid Transported-Tabulated Chemistry for Efficient Large Eddy Simulation of Turbulent Premixed Combustion”, Under Preparation, 2021.

External Conferences:

1. Application of Intrusive and Non-Intrusive Reduced Order Modeling Techniques for Simulation of Turbulent Premixed Flames, AIAA Propulsion and Energy Forum and Exposition, 2021 (Presenter: R. Ranjan).

2. Application of Hybrid Transported-Tabulated Chemistry for Efficient Large Eddy Simulation of Turbulent Premixed Combustion, AIAA SciTech Forum and Exposition, 2021 (Presenter: R. Ranjan).

Presentations at UTC:

1. Numerical Investigation of the Effects of Elevated Pressure and Chemistry on the Characteristics of Turbulent Premixed Flames, Research Dialogues, UTC, 2021 (Presenter: J Bowers).

2. Simulation of Extinction And Re-Ignition Events in a Turbulent Non-Premixed Flame, CECS Tech Symposium, UTC, 2021 (Presenter: J. Doshi).

3. Effect of Pressure on Heat Release and Curvature Statistics of Turbulent Premixed Flame, CECS Tech Symposium, UTC, 2021 (Presenter: J Bowers).

4. Large Eddy Simulation of the Volvo Bluff Body Flame Experiment, CECS Tech Symposium, UTC, 2021 (Presenter: E. Durant).

Inventions or Other Intellectual Property

In-house research code: AVF-LESLIE, UTCFOAM

Research Outreach & Collaboration

The research conducted under this effort has extended the collaboration with Georgia Tech researchers and has led to newer collaboration with a researcher from Purdue University.

EXTERNAL FUNDING

Proposal Submissions

1. Numerical investigation of effects of condensed and gas-phase finite-rate kinetics on the flame structure and surface regression in solid propellant combustion, White Paper, Propulsion, and Energetics Program, DEPSCOR, 2020.

2. A low emission combustion system for high overall pressure ratio compact core engines, Stage A Proposal, NASA ULI, 2020.

3. Reduced-Order Modeling Techniques for Efficient Simulation of Turbulent Combustion, 2021 ORAU Ralph E. Powe Junior Faculty Enhancement Awards, 2021.

Contracts/Awards Received

N/A

WHAT'S NEXT FOR THIS RESEARCH?

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

The PI is working on completing the journal paper submission. In addition, the PI will be submitting white papers and proposals, which will leverage the accomplishments of the project. In particular, the PI is planning to pursue three research directions in the next few years. These include (a) fundamental investigation of turbulence-chemistry interaction at elevated pressure with realistic fuels, (b) development and application of efficient approaches for the computation of chemistry while employing finite-rate kinetics, and (c) further development of ROM capabilities.

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

The work carried out under this research project has further established the ongoing collaboration of the PI with the researchers from Georgia Tech and Purdue, which will be extended further in the future. The goal of future collaborations will be to incorporate features of machine learning techniques, GPU computing to further enhance the efficiency of the current computational models and techniques, and to develop analysis tools for thermo-acoustic instabilities.

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

The PI did not experience any budget issues during the project. The remaining funds, if allowed, will be used to support graduate or undergraduate students.

Fiscal Year 2021 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (COVID-19 Research)

Michael Danquah, Lead PI

Other Personnel: Michael Danquah, Dr

Project Title: SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics

Date Report Submitted: October 23, 2020

Award Start – End Date: May 1, 2020 – September 30, 2020

Non-Technical Summary:

Covid-19 has recently been announced by WHO as a pandemic disease with pneumonia-like complications. It is caused by the novel coronavirus SARS-CoV-2 and has been spreading rapidly in various countries worldwide. Transmission of the virus to humans mostly occurs via respiratory droplets from symptomatic and asymptomatic patients, as well as artifacts contaminated with the virus. Currently, the techniques used for Covid-19 diagnosis include Reverse-T Polymerase Chain Reaction, Isothermal Nucleic Acid Amplification, and Blood-Based Serological Tests. Whilst these methods have somewhat been useful in supporting Covid-19 mitigation efforts, they are challenged by several factors including long turnaround times, lack of specificity, false negative/positive results, and exhaustive sample preparation steps, amongst others. There is an urgent need for more robust, fast, and precise methods for Covid-19 diagnosis.

The SARS-CoV-2 virus is constructed by the assemblage of 4 distinct structural proteins, namely S (Spike glycoprotein), E (Envelope protein), M (Membrane protein) and N (Nucleoprotein). The N protein plays a key role in protecting the viral genome and its replication, the viral host infection process, and alteration of the host's immune response, making it an important functional target for the development of Covid-19 therapeutics. This project investigated how unique nucleic acid molecules called aptamers can be engineered to bind to the RNA-binding domains (RBD) of the N protein. Such bioprobes will be useful for rapid detection of the virus with high precision as well as offer targeted delivery of therapeutics to fight the virus. In this project, we accomplished successful construction of the structural models of the N protein of the virus and investigated conditions that enable high-affinity binding of the N protein to the aptamer. This preliminary work has so far generated two extramural proposal submissions (one NSF and one NIH), and two journal articles which are currently under review. The funding also supported 1 PhD student.

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

Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH

This project is developing RNA aptamer probes to specifically target the RNA-binding domains (RBD) of SARS-COV-2 N protein. The approach is based on:

- Constructing structural models of the N protein.
- Performing MD simulations to study structural and binding conformational dynamics.
- Determining the specificity and stability of the aptamer-N protein complex.

OUTCOMES

The outcomes of this project so far includes

- 2 submitted proposals (NIH & NSF PI Danquah)
- 2 research manuscript under review
- Support for 1 PhD student

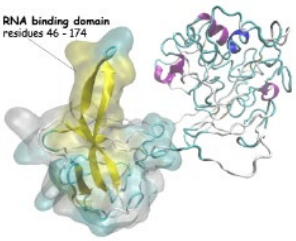

Fig. 2. Structure of SARS-COV-2 N protein showing the N terminal RBD.

RESULTS

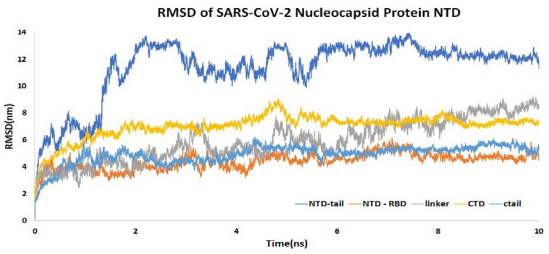

Fig 1. RMSD data of 10 ns MD simulation of SARS-CoV-2 N proteins showing the structural stability of the N terminal RBD compared other domains of the protein.

Structural modeling of the RBD of SARS-CoV-2 N protein showed that

- At pH 7.0 and temperature 310K, the RBD shows higher conformational stability when neutralized with 0.15 M Na^{+} compared to divalent Ca^{2+} and Na^{+}/Ca^{2+} combination.

OTHER INFO

Budget and Schedule

Total Budget:	$20,000
Actual Used:	$20,000
Balance:	$0

Total period of performance is 4 months.

Task 1: Months 1-5: Constructing structural models of the SARS-CoV-2 N protein.

Deliverables

- Successful construction of the structural models of the N protein of the virus and investigated conditions that enable high-affinity binding of the N protein to the aptamer
- 2 submitted proposals (NIH & NSF PI Danquah)
- 2 research manuscripts under review

• The RBD stability analysis indicates an optimal ionic strength condition for high-stability aptameric targeting of the N protein. • The stability of the RBD is important for optimal molecular docking and targeting of the N protein for theranostics application.	

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Covid-19 has recently been announced by WHO as a pandemic disease with pneumonia-like complications. It is caused by the novel coronavirus SARS-CoV-2 and has been spreading rapidly in various countries worldwide. Transmission of the virus to humans mostly occurs via respiratory droplets from symptomatic and asymptomatic patients, as well as artifacts contaminated with the virus. Currently, the techniques used for Covid-19 diagnosis include Reverse-T Polymerase Chain Reaction, Isothermal Nucleic Acid Amplification, and Blood-Based Serological Tests. Whilst these methods have somewhat been useful in supporting Covid-19 mitigation efforts, they are challenged by several factors including long turnaround times, lack of specificity, false negative/positive results, and exhaustive sample preparation steps, amongst others. There is an urgent need for more robust, fast, and precise methods for Covid-19 diagnosis.

The SARS-CoV-2 virus is constructed by the assemblage of 4 distinct structural proteins, namely S (Spike glycoprotein), E (Envelope protein), M (Membrane protein) and N (Nucleoprotein). The N protein plays a key role in protecting the viral genome and its replication, the viral host infection process, and alteration of the host's immune response, making it an important functional target for the development of Covid-19 therapeutics. This project will investigated the molecular mechanisms governing transformations in the structures and binding motifs of RNA aptamers via structural modeling and molecular dynamics (MD) simulations to target the RNA-binding domains of the N protein. Such bioprobes will be useful for rapid detection of the virus with high precision as well as offer targeted delivery of therapeutics to fight the virus. In this project, we accomplished successful construction of the structural models of the N protein of the virus and investigated conditions that enable high-affinity binding of the N protein to the aptamer. This preliminary work has so far generated two extramural proposal submissions (one NSF and one NIH), and two journal articles which are currently under review. The funding also supported 1 PhD student.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Constructing structural models of the N protein.	Developed initial N protein structures using PDB resources
Performing MD simulations to study structural and binding conformational dynamics.	MD simulations of the protein structure to establish RMSD stability characteristics
Determining the specificity and stability of the aptamer-N protein complex.	Evaluated biophysical conditions for binding stability

Challenges & Strategies Used to Address / Overcome:

No, however, there were some initial minor technical problems with running MD simulations on the cluster but this didn't impact the project significantly.

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 preliminary results from this project supported 2 external funding proposal submissions. If these proposals are funded, it will create more opportunities for the PI to expand the scope of work in this at UTC.

Students Impacted

The project supported 1 PhD student (Godfred Sabbih) during the summer.

Community and Broader Impacts

The project seeks to find ways to improve Covid-19 diagnosis, hence there is a huge community interest in the work. This project has the potential to create more collaborative opportunities with healthcare institutions in Chattanooga.

Scholarly Products

Publications:

1. Biophysical analysis of SARS-CoV-2 transmission and theranostic development via N protein computational characterization. Biotechnology Progress (Accepted for publication)
2. Engineered Aptamers for Enhanced COVID-19 Theranostics. Cellular and Molecular Bioengineering (Under Review)

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

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

1. Wireless electrochemical aptasensing of SARS-CoV-2 nucleoproteins for rapid Covid-19 diagnosis and telehealth applications. NIH R15. Lead PI
2. Collaborative Research: RUI: Spike protein and ACE2 binding checkpoint for rapid screening of SARS-CoV-2 from saliva via nanostructured bijeltemplated electrochemical biosensor. NSF RUI. Lead PI

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 wish to look for more opportunities to attract external funding to extend this project.

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

N/A

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

N/A

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

N/A

FINANCIAL ACCOUNTING

N/A

Fiscal Year 2021 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (COVID-19 Research)

Lead PI: Dr. Soubantika Palchoudhury

Co-PI(s): Prof. Abdollah Arabshahi

Project Title: "Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19"

Date Report Submitted: 12/6/2020

Award Start – End Date: May 1, 2020 – September 30, 2020

Non-Technical Summary:

Please provide a non-technical summary of your project that addresses the major objectives, accomplishments, and outcomes of your project. Discuss impacts of the project in terms of scholarly contributions to the field, scholarly outputs, student and community impacts, etc. Address how your project advanced or supported the mission of the SimCenter.

A new panic zone RNA virus, severe acute respiratory syndrome coronavirus (SARS-CoV-2), has triggered the global pandemic of COVID-19, a pneumonia-like respiratory infection that has caused nearly one million deaths worldwide and has devastated the global economy. One of our key defenses against this deadly viral spread is early detection through testing and isolation of positive cases. SARS-CoV-2 can show an incubation period of 24 days and the virus can spread through asymptomatic individuals. This makes testing a priority to combat this pathogen. A point-of-care diagnostic test for COVID-19 will be a breakthrough innovation for our society, particularly for rural areas without adequate healthcare facilities. Current diagnostics for SARS-CoV-2 rely on reverse transcription polymerase chain reaction, immunoassays, and computed tomography. In this project, we aimed to realize a new and cost-effective point-of-care assay of high specificity and sensitivity for SARS-CoV-2. We designed this point-of-care assay by synthesizing novel biohybrid gold nanoparticle detection kit coupled with computational fluid dynamics predictions for suitable analyte concentrations. This flexible lateral flow paper assay will be further engineered as a pH-paper like colorimetric detection platform for the pathogen with a capability of result transmission via cellphone.

COMPUTATIONAL FLUID DYNAMIC APPROACH FOR POINT-OF-CARE DIAGNOSTICS WITH AU NANOPARTICLES FOR COVID-19

Technology Area of Interest: HEALTH AND BIOLOGICAL SYSTEMS

TECHNICAL APPROACH

Our goal was to realize a cost-effective and highly sensitive new point-of-care diagnostic tool for SARS-CoV-2 using engineered gold nanoparticles (NPs). This was achieved through the following approaches:

- *Synthesis and characterization of Au NPs*
- *Conjugation of SARS-CoV-2 spike proteins with Au NPs.*
- *Detection of SARS-CoV-2 via analyzing changes in absorbance profile of NPs.*
- *Designing a flexible paper-based diagnosis*
- *Investigating the influence of NP properties on the detection assay via CFD.*

OUTCOMES

We successfully engineered ligand coated and uncoated gold nanoparticles of different sizes and demonstrated a spectroscopic detection method for their binding with biomolecules. We will translate this to SARS-CoV-2 spike proteins in our next phase of studies. This project led to research training for two undergraduate students and financial support for one graduate student. One external conference presentation and two proposal submissions for external funding also resulted from this mini seed grant.

RESULTS

Four different Au NP formulations were successfully synthesized for the assay. Size and absorbance profile of NPs analyzed. Structure-property relations of the Au NPs were realized through multi-modal material characterization. Figure 1 shows a summary of our primary findings from the project.

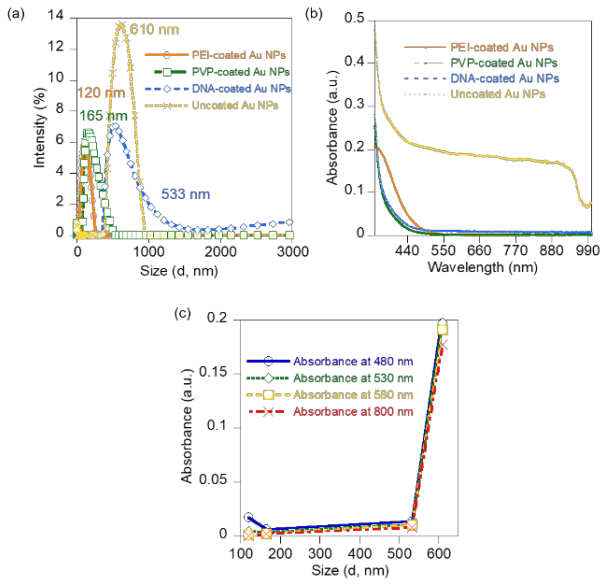

Figure 1. Size and ligand-dependent absorbance of Au NPs. (a) DLS size plots, (b) UV-vis plots, and (c) variation in the absorbance profile of Au NPs.

OTHER INFO

Budget and Schedule

Total Budget:	$ 20,000
Actual Used:	$ 20,000
Balance:	$ 0

Total period of performance is 4 months.

Task 1: Student recruitment, purchasing chemicals, synthesis of nanoparticles

Task 2: Attachment of biomolecules, mid-term report, proposal submission

Task 3: Spectroscopic detection

Task 3: Proposal submission, external conference presentation, final report

Deliverables

- Monthly report describing numerical methods, techniques, and results that were developed.
- Final report detailing results, financials, and future work was developed.
- 2 proposals were submitted.
- 1 external conference presentation at Virtual MRS 2020 Meeting

Organization Information

Dr. Soubantika Palchoudhury (PI), Civil and Chemical Engineering, University of Tennessee at Chattanooga (UTC), Phone: 423-425-5455, E-mail: soubantika-palchoudhury@utc.edu

Prof. Abdollah Arabshahi (co-PI), SimCenter, UTC, E-mail: Abi-Arabshahi@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Provide a scientific / technical overview of your research project – hypothesis or scientific aims, methodologies and activities, outcomes, etc. Length: up to 1 page

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Engineering gold NPs for detection	Development of a nanoparticle based point of care assay for detection of biomolecules
Characterization of NPs via dynamic light scattering and ultraviolet-visible spectroscopy	Submission of two external proposals
Attachment of different biomolecules on the NPs	One external conference presentation
Detection of biomolecules via spectroscopic analysis	
Proposal submission, report writing, and conference presentation	

Challenges & Strategies Used to Address / Overcome:

N/a

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

Goals were met

IMPACT & OUTCOMES

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

This project helped the PI in establishing a new research thrust in materials science based technologies for detection of infectious pathogens.

Students Impacted

1. Syed Mohammad Tareq, Ph.D. student, summer stipend and research experience, expected graduation: 2023
2. Dell Zimmerman, Chemical Eng. undergraduate student, research training, graduation: 2021
3. Gitapun Jur, Chemical Eng. undergraduate student, summer research, graduation: 2023

Community and Broader Impacts

This technology will be a groundbreaking advancement for our healthcare system as it will enable reliable detection of SARS-CoV-2 onsite without the need for expensive laboratory facilities. The technology will be most useful in remote or rural locations without advanced healthcare facilities.

Scholarly Products

External Conferences:

1. Oral talk at Materials Research Society Annual Conference, Virtual Meet, 2020 by the PI.

Inventions or Other Intellectual Property

Please consider and include new software products that are subject to copyright but also methods and systems are potentially patentable. If you filed invention disclosures or patent or copyright applications during the period of performance, please indicate so here as well. If you wish to open source a software prototype data set, please state so. We will follow up with you with a disclosure process and guidance on how to proceed effectively for UTC and our research program, including required preparation and how properly to credit ownership to the UT system.

N/a

Research Outreach & Collaboration

Detail new, continued, or expected collaborations as a result of this project, with names as appropriate. Also, please list any visitors, workshops, or other collaborative events you held. Indicate the location (on campus, etc.).

Established collaboration with Nanomaterials Theory Institute, Oak Ridge National Laboratory.

EXTERNAL FUNDING

Proposal Submissions

1. Investigating the dynamics and therapeutics for SARS-CoV-2 through an integrated computational and experimental approach, American Lung Association, $200,000
2. Investigating the dynamics and therapeutics for SARS-CoV-2 through an integrated computational and experimental approach, National Institute of Allergy and Infectious Diseases, $137,500

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?

This project will help me in establishing and leading a niche research area for novel point-of-care diagnostics and flexible bioelectronics for infectious diseases using materials science.

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

I also plan on synthesizing new band-gap controlled semiconductor materials from earth-abundant elements using ab initio computation and experimental nanochemistry techniques.

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

Please explain any remaining funds, if applicable, or any budget issues you encountered in the project period.

All funds were used during the project.

Fiscal Year 2021 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in 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 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

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 tools based on machine learning	We accomplished the following: 1. Data on artiodactyl group sizes collected for ~200 populations. 2. 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). 3. Wang developed a mathematical model using data provided by Pope. 4. Azad Hossain and student extracted rainfall data for >10 years from the online database (CRU). This project will be completed Summer 2021. *5.* 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.	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: $67,528.33 Balance: $31,133.67 Total period of performance is 12 months. **Deliverables** • Quarterly reports describing progress and challenges • Final report detailing results, financials, and future work • Paper submitted to Journal of Mammalogy • UTC Research Dialogues presentation

	• External conference presentation (Evan Suggs) **Organization Information** *Departments of Biology, Geology, and Environmental Science and 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 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.
7. Connected CEACSE funded research to Hayes' NSF IRES program.

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, and added life history data from primary literature
Life history analysis	Compared data from primary literature to online database and conducted statistical analysis
Rainfall dataset	Used GPS locations from artiodactyl dataset, we are now extracting 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) is collaborating with Schradin (France). The student is funded by Hayes' NSF IRES program.
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 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 did not work? What did you disprove or learn from the parts that did not 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 new avenues of research with colleagues in math and geology.

Pope left the M.S. program after one year. Losing her will create some challenges (lost project memory, continuity). However, Hayes continues to communicate with her about her work and she has shared information freely with Hayes and collaborators. Funding is available for a new student in 2022.

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 is an Assistant Professor. Hayes could act as a mentor-collaborator.

Students Impacted

1. **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.
2. **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.
3. **Braxton Azalone** – Geology, undergraduate: Azalone is working on a rainfall dataset in Summer 2021. He plans to graduate in 2022.

4. **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.
5. **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.

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 by experiences. 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 the 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:

1. Olivier, C, Jaeggi, A., Hayes, L.D., & Schradin, S. Revisiting Macroscelidea social systems: Evidence for variable social organization, including pair-living, but not for a monogamous mating system. Submitted to Journal of Mammalogy.

External Conferences:

1. Suggs, E.D. 2019. Meta-textual analysis of biological research. ACM meeting, Gatlinburg, TN.
2. 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:

1. 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 is using 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 coordinated 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 Sept 2021. This activity will become part of a broader impacts section of a NSF proposal.
https://www.socialevolutionseminar.com

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

1. Consultations with NSF IRES program officer.
2. 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 have 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 are interacting with personnel 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.

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 will use some of the funds to support a graduate student in Spring 2022.

Fiscal Year 2021 Final Project Report

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

Osama A. Osman, Lead PI

Co-PI(s): Farah Kandah

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, 2021

Non-Technical Summary:

Summary: The proposed research includes modeling, simulation, and computational performance analytics and optimization. The proposed research aims to apply of 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 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 facilitate experimental research and training in highly controllable conditions. Additionally, the integrated platform will 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 will add a high-degree of realism since assumptions and mathematical models of road user behaviors will not be the basis of simulation. The proposed platform will also enable subjective feedback (e.g. emotions) of road users in addition to objective parameters (e.g. actual actions). The proposed work will be collaboratively conducted by Principal Investigators (PIs) with extensive and complimentary 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.

Accomplishments and Outcomes:

The research team finished the literature review and was able to identify similar projects and their limitations, which the team is working to overcome in the project herein. The team purchased all the required equipment for the project and began working on the simulator

software to develop the simulation scenarios and the analytics tools. Additionally, the team has acquired the required equipment to add a pedestrian in the simulation loop. In the meantime, the team is researching optimal ways to develop the proposed integration herein.

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

Technology Area of Interest: CUIP

TECHNICAL APPROACH	OUTCOMES
• *List of tasks* 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 is currently in the process of purchasing a computer to be dedicated to the HMD as we realized that the simulator computer may not take the computational loads of both pieces of equipments. The team is currently working on the development and integration process.
RESULTS	**OTHER INFO**
None yet.	**Budget and Schedule** Total Budget: $99,998.00 Actual Used: $85,170.82 Balance: $14,827.18 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: 423-425-4398; Osama-osman@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Nothing to report at this stage.

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 PIs request, the award start date was pushed backwards to January 1st, 2021 instead of July 1st, 2020 due to 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.

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

Nothing to report

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.

Community and Broader Impacts

Nothing to report yet.

Scholarly Products

Publications:

1. Nothing to report yet.

External Conferences:

1. Nothing to report yet.

Presentations at UTC:

1. Nothing to report yet.

Inventions or Other Intellectual Property

Nothing to report yet.

Research Outreach & Collaboration

Nothing to report yet.

EXTERNAL FUNDING

Proposal Submissions

1. The team is in the process of submitting a research needs statement to Tennessee Department of Transportation that builds on the integrated platform being developed in this project.

Contracts/Awards Received

Nothing to report yet.

Sponsored Program Capacity Building Activities

1. 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

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

Nothing to report.

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

Developing the integration is a challenging process. We are communicating with the simulator developers and other researchers to get any required input. The purchase of the equipment was severly delayed due to COVID and hiring a graduate student was a more challenging process due to the same reason. We are currently working to make up for the delays caused by these challenges.

FINANCIAL ACCOUNTING

Remaining is $17,128.11 which is used to purchase the computer and to cover an undergraduate and graduate student salaries.