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

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Submitted by
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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


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.


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 Amir Kabir 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.

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*, *Behavioral Ecology and Sociobiology*, *Biological 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 Palchoudhury

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

Lead PI: “Computational Fluid Dynamic Approach 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.


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.


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”
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.

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

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<thead>
<tr>
<th>Lead PI</th>
<th>Project Title</th>
<th>CEACSE Priority Area</th>
<th>Amount Awarded</th>
<th>Amount Expended</th>
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<tbody>
<tr>
<td>Reetesh Ranjan</td>
<td>An Efficient Framework for Numerical Investigation of Turbulent Combustion using Detailed Finite-Rate Chemistry</td>
<td>Advanced Modeling &amp; Simulation</td>
<td>$76,099</td>
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<td>Eleni Panagiotou</td>
<td>Topological design of porous metals for biomedical applications</td>
<td>Health &amp; Biological Systems</td>
<td>$99,941</td>
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<td>Osama Osman</td>
<td>Development of an Integrated Human-in-the-Loop Simulation Platform for Smart City Applications</td>
<td>Smart Cities &amp; Urban Dynamics</td>
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<td>$87,171**</td>
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<td>Loren Hayes</td>
<td>Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models</td>
<td>Health &amp; Biological Systems</td>
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<td>Vahid Disfani</td>
<td>Real-Time Optimal Allocation of Adaptive Virtual Inertia in Power Systems with High Penetration of Distributed Energy Resources</td>
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<td>Andrew Bailey</td>
<td>People, planet, and profits: Strategic planning for outdoor recreation, tourism and conservation</td>
<td>Environment</td>
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<td>Abi Arabshahi</td>
<td>Enhanced Eulerian-Lagrangian Formulation for Investigation of Turbulent Dispersed Multiphase flows</td>
<td>Advanced Modeling &amp; Simulation</td>
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## NEW INITIATION/OPPORTUNITY AWARDS FY2021

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<td>Yunye Shi</td>
<td>Predicting biomass gasification output: A machine learning approach</td>
<td>Energy</td>
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<td>A Topological Analysis of Viral Glycoproteins-Application to the Spike Protein of SARS-CoV-2</td>
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<td>Michael Danquah</td>
<td>SARS-CoV-2 Nucleocapsid Protein Targeting for Enhanced Covid-19 Theranostics</td>
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<td>Soubantika Palchoudhury</td>
<td>Computational Fluid Dynamic Approach for Point-of-Care Diagnostics with Au Nanoparticles for COVID-19</td>
<td>Health &amp; Biological Systems</td>
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** 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

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<th>Total Revenue</th>
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### Expenditures

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### Centers of Excellence - Actual, Proposed, and Requested Budget

- **Engineering**
- **Computer Science**

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Institution: UT Chattanooga
FY2021 PUBLICATIONS AND PRESENTATIONS
(of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings


“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)


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

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, “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 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)


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, “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


Contracts/Awards Received


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

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

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<td>PI</td>
<td>No</td>
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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


### Contracts/Awards Received
N/A

### Sponsored Program Capacity Building Activities
N/A

<table>
<thead>
<tr>
<th>Michael Danquah, Lead PI</th>
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</thead>
</table>

**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

<table>
<thead>
<tr>
<th>Dr. Soubantika Palchoudhury, Lead PI</th>
</tr>
</thead>
</table>

**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 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.

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 and 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

c. Products
(i) 5 Selected Products (*Student Author)

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


d. Synergistic Activities

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


5. Faculty Advisor, UTC Student Chapter, National Society of Black Engineers (NSBE), 2016-present.
ABDOLLAH (ABI) ARABSHAHI
Research Professor | SimCenter and Computational Science and Engineering
University of Tennessee at Chattanooga | Chattanooga, TN 37403
Tel: 423-425-5485, Fax: 423-425-5517, Email: Abi-arabshahi@utc.edu

A. Professional Preparation:

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

B. Appointments:

2005 – Present
Research Professor
University of Tennessee at Chattanooga

2002 – 2005
Associate Research Professor
University of Tennessee at Chattanooga

1997 – 2002
Senior Research Associate
Applied Research Laboratory, The Pennsylvania State University

1995 – 1997
Research Engineer II, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University

1991 - 1995
Research Engineer I, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University

1989 – 1991
Post-doctoral Fellow, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University

C. Selected Recent Publications

i) Five publications most closely related to proposed project:

ii) Five other significant publications:

- 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.

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 4 PhD 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
518 Oak Street, Chattanooga, TN 37403
423-290-6142
Andrew-Bailey@utc.edu

(a) Professional Preparation

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<th>Degree</th>
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<td>Knoxville, TN</td>
<td>Theology/Education</td>
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<td>University of Tennessee</td>
<td>Knoxville, TN</td>
<td>Rec. Parks. Tourism</td>
<td>M.S. 1999</td>
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<tr>
<td>University of Minnesota</td>
<td>Minneapolis, MN</td>
<td>Education</td>
<td>Ph.D. 2009</td>
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(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


Other Products


(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 HHIP & 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.

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

Vahid Disfani
University of Tennessee at Chattanooga
Department of Electrical Engineering
Phone: 423-425-4354 Fax: 423-425-5229 Email: vahid-disfani@utc.edu

(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

(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

<table>
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<tr>
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<tr>
<td>Bates College (Maine)</td>
<td>Biology</td>
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<td>1992-1996</td>
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<td>Michigan State University</td>
<td>Zoology</td>
<td>M.S.</td>
<td>1996-1999</td>
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<td>Miami University (Ohio)</td>
<td>Zoology</td>
<td>Ph.D.</td>
<td>2000-2004</td>
</tr>
</tbody>
</table>

B. Appointments

<table>
<thead>
<tr>
<th>Year</th>
<th>Position</th>
<th>Institution</th>
</tr>
</thead>
<tbody>
<tr>
<td>2014-present</td>
<td>Associate Professor</td>
<td>University of Tennessee at Chattanooga</td>
</tr>
<tr>
<td>2015</td>
<td>Visiting Scholar</td>
<td>USIAS, Strasbourg, France</td>
</tr>
<tr>
<td>2012-2014</td>
<td>Assistant Professor</td>
<td>University of Tennessee at Chattanooga</td>
</tr>
<tr>
<td>2010-2011</td>
<td>Associate Professor</td>
<td>University of Louisiana at Monroe</td>
</tr>
<tr>
<td>2007-2009</td>
<td>Visiting Professor</td>
<td>Universidad Austral de Chile</td>
</tr>
<tr>
<td>2004-2010</td>
<td>Associate Researcher</td>
<td>P. Universidad Católica de Chile</td>
</tr>
<tr>
<td>2004-2010</td>
<td>Assistant Professor</td>
<td>University of Louisiana at Monroe</td>
</tr>
</tbody>
</table>

C. Products

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


(ii) Five other products (*=student)


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

Guerry Professor
Department of Health and Human Performance
The University of Tennessee at Chattanooga
Phone: (423) 425-4432, Fax: (423) 425-4457
Email: Gregory-Heath@utc.edu

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.

RC. Evidence-based intervention in physical activity: lessons from around the world. Lancet
2012; 380:272-81.

Progress in physical activity over the Olympic quadrennium. Lancet. 2016 Jul 27. pii: S0140-

[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

Other Significant Products


Complete List of Published Work in MyBibliography:

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

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

Awards
  o Delta Omega, Kappa Chapter (Honorary Public Health Society)
  o Elected to Alpha Society, University of Tennessee at Chattanooga Academic Honor Society (2006)
Hamdy Ibrahim  
University of Tennessee at Chattanooga (UTC)  
Department of Mechanical Engineering  
Tel: 423-425-4718, Fax: 423-425-5229, Email: hamdy-ibrahim@utc.edu

(a) Professional Preparation

<table>
<thead>
<tr>
<th>Institution</th>
<th>City</th>
<th>Country</th>
<th>Field</th>
<th>Degree</th>
<th>Year</th>
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<tbody>
<tr>
<td>Cairo University</td>
<td>Cairo</td>
<td>Egypt</td>
<td>Mechanical Engineering</td>
<td>B.S.</td>
<td>2008</td>
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<tr>
<td>Cairo University</td>
<td>Cairo</td>
<td>Egypt</td>
<td>Mechanical Engineering</td>
<td>M.S.</td>
<td>2012</td>
</tr>
<tr>
<td>The University of Toledo</td>
<td>Toledo</td>
<td>OH</td>
<td>Mechanical Engineering</td>
<td>Ph.D.</td>
<td>2017</td>
</tr>
<tr>
<td>The University of Toledo</td>
<td>Toledo</td>
<td>OH</td>
<td>Mechanical Engineering</td>
<td>2017-18</td>
<td>Postdoc</td>
</tr>
</tbody>
</table>

(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:


(ii) Five other significant publications:

- **Ibrahim, H.,** Dehghanhadikolaei, 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.


(d) **Patents**

• **Ibrahim, H.** and Elahinia, M. Heat Treatment Process to Produce High Strength and Corrosion Resistance Mg-Ca-Zn Alloy for Patient-Specific Bioreorable Bone Fixation Hardware. US2019001027A1, December 21, 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  
GIS Director  
701 E M L King Blvd, Chattanooga, TN 37403  
423-635-2239  
Charles-mix@utc.edu https://www.utc.edu/research-sponsored-programs/interdisciplinary-geospatial-technology-laboratory

(a) Professional Preparation

<table>
<thead>
<tr>
<th>University</th>
<th>Location</th>
<th>Major</th>
<th>Degree</th>
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<tr>
<td>Jacksonville State University</td>
<td>Jacksonville, AL</td>
<td>Geography</td>
<td>Bachelor of Science 2009</td>
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(b) Appointments

<table>
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<tr>
<th>Year</th>
<th>Position</th>
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<tr>
<td>2018 - Present</td>
<td>Geographic Information Systems (GIS) Director, University of Tennessee Chattanooga, Chattanooga, TN, USA</td>
</tr>
<tr>
<td>2015 - 2018</td>
<td>Geographic Information Systems (GIS) Manager, University of Tennessee Chattanooga, Chattanooga, TN, USA</td>
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<tr>
<td>2013 – 2014</td>
<td>Interim Executive Director, North Chickamauga Creek Conservancy, Hixson, TN US</td>
</tr>
<tr>
<td>2013 – 2014</td>
<td>Interim Executive Director, North Chickamauga Creek Conservancy, Hixson, TN US</td>
</tr>
<tr>
<td>2012 -2014</td>
<td>GIS Coordinator, North Chickamauga Creek Conservancy, Hixson, TN, USA</td>
</tr>
<tr>
<td>2010 – 2011</td>
<td>Conservation Planner, North Alabama &amp; Georgia Land Trust, Piedmont, AL, USA</td>
</tr>
<tr>
<td>2010 - 2011</td>
<td>Research Assistant, National Park Service-Russell Cave National Monument, Bridgeport, AL, USA</td>
</tr>
</tbody>
</table>

(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:
2. **2017 3D Mapping of Chattanooga, TN**
   Using Light Detection and Ranging Data (Lidar) 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/apps/Styler/index.html?appid=591f643addb5474c9ab321d80a00543c

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

**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 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
Visiting Researcher, Swiss Federal Institute of Technology ETH Zurich, 2011–2012

Five publications most closely related to the proposed project


Five other significant publications


**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
(a) Professional Preparation

<table>
<thead>
<tr>
<th>Institution</th>
<th>Location</th>
<th>Degree(s)</th>
</tr>
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<tbody>
<tr>
<td>University of Illinois</td>
<td>Urbana-Champaign, IL</td>
<td>Theoretical &amp; Applied Mechanics MS (2009), PhD (2012)</td>
</tr>
<tr>
<td>Georgia Institute of Technology</td>
<td>Atlanta, GA</td>
<td>Aerospace Engineering 2013-2015</td>
</tr>
</tbody>
</table>

(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

(c) Products


(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.


(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

(d) Synergistic Activities

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


(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).

Biographical Sketch

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

(a) Professional Preparation

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

(b) Appointments

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

(c) Publications

(i) Most Closely Related Products

1. L Zhao, B Bhatia, S Yang, E Strobach, LA Weinstein, TA Cooper, EN Wang, Harnessing Heat Beyond 200° C from Unconcentrated Sunlight with Non-Evacuated Transparent Aerogels, ACS Nano, 2019, 13 (7), 7508
2. E Strobach, B Bhatia, S Yang, L Zhao, EN Wang, High temperature stability of transparent silica aerogels for solar thermal applications, APL Materials, 2019, 7 (8), 081104
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

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
5. A Rieth, S Yang, E Wang, M Dinca, Record Atmospheric Fresh Water Capture

(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 (PND) 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 plotted 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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
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</table>
| 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. |

<table>
<thead>
<tr>
<th>RESULTS</th>
<th>OTHER INFO</th>
</tr>
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</table>
| 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. | **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 |

Streamwise velocity fluctuations 5 step-heights downstream from step feature after 24 flow-through times
ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

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.


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


Contracts/Awards Received

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
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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
</table>
| 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. |

<table>
<thead>
<tr>
<th>RESULTS</th>
<th>OTHER INFO</th>
</tr>
</thead>
</table>
| 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: Months 10-12 Publication preparation |
### ACCOMPLISHMENTS & OUTCOMES

#### Project Overview

<table>
<thead>
<tr>
<th>List of Objectives / Aims / Major Milestones</th>
<th>Cumulative Outcomes / Accomplishments</th>
</tr>
</thead>
<tbody>
<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>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 &quot;if-else&quot; 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>
<td></td>
</tr>
<tr>
<td>SVM model</td>
<td></td>
</tr>
<tr>
<td>SVM model with polynomial kernel</td>
<td></td>
</tr>
<tr>
<td>SVM model with radial kernel</td>
<td></td>
</tr>
<tr>
<td>Regularized regression model</td>
<td></td>
</tr>
</tbody>
</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 CO₂ neutral, less NOₓ 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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
<tbody>
<tr>
<td>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:</td>
<td>2 conference papers:</td>
</tr>
<tr>
<td>• Task 1. Investigating VI and VD Provision of Different DER Technologies</td>
<td>• 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.</td>
</tr>
<tr>
<td>• Task 3. Real-Time Digital Simulation Implementations</td>
<td>1 presentation in UTC ReSEARCH Dialogue</td>
</tr>
<tr>
<td></td>
<td>• P. Ubiratan, “Distributed Inter-Area Oscillation Damping Control Via Dynamic Average Consensus Algorithm,” in UTC ReSEARCH Dialogues.</td>
</tr>
<tr>
<td></td>
<td>1 MS Thesis</td>
</tr>
<tr>
<td></td>
<td>• 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.</td>
</tr>
</tbody>
</table>
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

<table>
<thead>
<tr>
<th>List of Objectives / Aims / Major Milestones Proposed</th>
<th>Cumulative Outcomes / Accomplishments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Task 1. Investigating VI and VD Provision of Different DER Technologies</td>
<td>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.</td>
</tr>
<tr>
<td>Task 2. Developing Real-Time Adaptive VI/VD Allocation</td>
<td>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.</td>
</tr>
<tr>
<td>Task 3. Real-Time Digital Simulation Implementations</td>
<td>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.</td>
</tr>
</tbody>
</table>

### 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/](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:


**External Conferences:**


**Presentations at UTC:**


**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**


**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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
<tbody>
<tr>
<td>The major milestones include:</td>
<td>The research outcomes include:</td>
</tr>
<tr>
<td>1. Finalized synthetic method of OTTI aerogel</td>
<td>1. Won Ruth S. Holmberg Grant</td>
</tr>
<tr>
<td>2. Optimizing chemical recipes for ambiently dried aerogel</td>
<td>2. Submitted NSF-ERI proposal, $200k (in review)</td>
</tr>
<tr>
<td>3. RTE and Mie theory modeling</td>
<td>3. In progress (~50%), a peer-reviewed publication on ambiently-dried aerogel</td>
</tr>
<tr>
<td>5. Solar process heat generator design &amp; modeling</td>
<td></td>
</tr>
</tbody>
</table>

### RESULTS
Please, see the attached research report for the details

### OTHER INFO

**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)
ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

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 amount of efforts to conduct various experiments and theoretical 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:


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.

<table>
<thead>
<tr>
<th>Proposal name</th>
<th>PI or co-PI</th>
<th>External?</th>
<th>Amount requested</th>
<th>Cayuse #</th>
</tr>
</thead>
<tbody>
<tr>
<td>NSF-ERI</td>
<td>PI</td>
<td>Yes</td>
<td>199980</td>
<td>21-4830</td>
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<tr>
<td>ENV-SMART</td>
<td>Co-PI</td>
<td>Yes</td>
<td>443405</td>
<td>21-4466</td>
</tr>
<tr>
<td>NSF_MRI</td>
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<td>Yes</td>
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<td>TVA</td>
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<td>21-1225</td>
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<tr>
<td>Ruth S. Holmberg</td>
<td>PI</td>
<td>No</td>
<td>5000</td>
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</tr>
</tbody>
</table>

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.

<table>
<thead>
<tr>
<th>Description</th>
<th>1</th>
<th>2</th>
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<tbody>
<tr>
<td>Finalizing synthetic method of OTTI aerogel (10x10cm²)</td>
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<tr>
<td>Optimizing chemical recipes for ambient dried aerogel</td>
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<tr>
<td>Optical &amp; thermal modeling via RTE and Mie theory</td>
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<tr>
<td>Mechanical modeling via molecular dynamics</td>
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<tr>
<td>Building solar collector assembly &amp; lab testing</td>
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<td>Solar process heat generator design &amp; modeling</td>
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<tr>
<td>Constructing the solar process heat generator assembly</td>
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<td>Integrating PCM thermal storage in the heating loop</td>
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<td>Outdoor experiments with the final prototype</td>
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<tr>
<td>Finalizing commercialization plan and form partnerships</td>
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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:](image)

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.](image)

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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
</table>
| • 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., Irl, 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

<table>
<thead>
<tr>
<th>RESULTS</th>
<th>OTHER INFO</th>
</tr>
</thead>
</table>
| **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.

<table>
<thead>
<tr>
<th>List of Objectives / Aims / Major Milestones Proposed</th>
<th>Cumulative Outcomes / Accomplishments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Creation of a new measure of local topology of proteins</td>
<td>Created and submitted for publication</td>
</tr>
<tr>
<td>Topological analysis of SARS-CoV-2 and other viral proteins</td>
<td>Completed and submitted for publication</td>
</tr>
</tbody>
</table>

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)
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


**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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
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<tbody>
<tr>
<td>Three-year visitation estimates were established using cell phone tracking data.</td>
<td>Working partnerships with local, regional, and state entities.</td>
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<tr>
<td>These estimates informed valuation of park spaces through IMPLAN tourism economic</td>
<td>Multiple models illustrating the recreational, health, and conservation</td>
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<tr>
<td>impact multipliers, CDC burden of disease indicators, and environmental mitigation</td>
<td>values of regional green spaces.</td>
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<td>data. Combined data were mapped and analyzed with optimal hot spot analyses, a</td>
<td>Three presentations, including one recognized as a top three of the</td>
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<td>machine learning process that identifies spatially significant clusters of hot</td>
<td>conference proceedings.</td>
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<td>and cold spots based on given criteria.</td>
<td>Multiple presentations, manuscripts, and a grant proposal in progress.</td>
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<td>New lines of research based on the influence and opportunity afforded by</td>
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<td>green space during the COVID pandemic.</td>
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<td>More than 70 students impacted as data collectors, analysts, and presenters of research.</td>
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<tr>
<th>RESULTS</th>
<th>OTHER INFO</th>
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<tbody>
<tr>
<td>See Appendices for Tables and Figures.</td>
<td>Budget and Schedule</td>
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<tr>
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<td>Total Budget:                 $76,577</td>
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<td>Actual Used:                  $51,681.82</td>
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<td>Balance:                      $24,895.18</td>
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<td>Total period of performance is 12 months.</td>
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<td>Task 1: Staff hired, survey &amp; field data collected, big data sorted, GIS</td>
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<td>Task 2: Sorting big data &amp; combining data for analyses.</td>
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<td>Task 3: Merging data geospatially and conducting preliminary analyses.</td>
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<td>Task 3: Iterative GIS-based analyses for optimal outcome reporting.</td>
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<td>Deliverables                 UTC HHP: <a href="mailto:Andrew-Bailey@utc.edu">Andrew-Bailey@utc.edu</a></td>
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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.
<table>
<thead>
<tr>
<th>List of Objectives / Aims / Major Milestones Proposed</th>
<th>Cumulative Outcomes / Accomplishments</th>
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</thead>
<tbody>
<tr>
<td>Goal 1: To establish a baseline and trend of recreation usage in the Thrive Region.</td>
<td>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).</td>
</tr>
<tr>
<td>Goal 2: To establish a baseline and forecast trends of environmental impacts of recreational use.</td>
<td>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.</td>
</tr>
<tr>
<td>Goal 3a: To estimate economic values of natural areas in the region based on tourism expenditures.</td>
<td>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.</td>
</tr>
<tr>
<td>Goal 3b: To estimate economic values of natural areas based on preventive health and prevention of environmental mitigation.</td>
<td>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.</td>
</tr>
<tr>
<td>Goal 4: To forecast the impacts of increased development, increased usage, and climate change on environmental values.</td>
<td>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.</td>
</tr>
<tr>
<td>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.</td>
<td>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.</td>
</tr>
<tr>
<td>Additional findings: Impacts of COVID on visitation to regional parks and green spaces.</td>
<td>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.</td>
</tr>
</tbody>
</table>
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:**


**Presentations at UTC:**


**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.
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.

<table>
<thead>
<tr>
<th>County</th>
<th>Multiplier</th>
<th>Daily Total Impact</th>
<th>2019 Visitation (Sample)</th>
<th>Total Impact</th>
<th>State Taxes</th>
<th>Fed Taxes</th>
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</table>

The Chattanooga region is renowned 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.

<table>
<thead>
<tr>
<th>County</th>
<th>Tourism Revenue</th>
<th>Air Mitigation</th>
<th>Water Mitigation</th>
<th>Health Values (Park Space)</th>
<th>%15yr Development</th>
<th>Total CC Visit Loss</th>
<th>Annual Tourism Loss to CC (2060)</th>
<th>Annual Mitigation Loss (2060)</th>
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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.
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.
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.
References


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

<table>
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<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Establish finite-rate chemistry-based strategy for simulation of turbulent</td>
<td>• Established tools and models for simulation of turbulent combustion</td>
</tr>
<tr>
<td>combustion using high-performance computing (HPC) tools</td>
<td>in canonical and applied configurations</td>
</tr>
<tr>
<td>• Implement HTTC and ROM techniques</td>
<td>• Trained 2 graduate students and 1 undergraduate student on simulation</td>
</tr>
<tr>
<td>• Implement subgrid models for LES</td>
<td>of turbulent combustion using HPC tools and analysis of results using</td>
</tr>
<tr>
<td>• Perform DNS and LES of turbulent premixed flames at elevated pressure and</td>
<td>Python, Tecplot, and Paraview</td>
</tr>
<tr>
<td>turbulent non-premixed jet flame to examine extinction and reignition</td>
<td>• Resulted into 1 MS thesis, 2 international conference articles, 2</td>
</tr>
<tr>
<td>• Develop tools for statistical and spectral analysis of turbulent premixed</td>
<td>international conference presentations, 4 internal conference presentations,</td>
</tr>
<tr>
<td>flames</td>
<td>2 journal articles under preparation, and 3 white papers/proposals</td>
</tr>
<tr>
<td>• Establish UTCFoam (an extended version of OpenFoam) for combustion simulations</td>
<td></td>
</tr>
<tr>
<td>• Analyze thermo-acoustics combustion instabilities</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>RESULTS</th>
</tr>
</thead>
</table>

**Budget and Schedule**

<table>
<thead>
<tr>
<th>Budget</th>
<th>Schedule</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Budget: $76,099.00</td>
<td>Actual Used: $67,977.91</td>
</tr>
<tr>
<td>Balance: $8,121.09</td>
<td>Total period of performance is 12 months with multiple tasks spread out during the entire year.</td>
</tr>
</tbody>
</table>

**Deliverables**

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

**Organization Information**

Department of Mechanical Engineering
University of Tennessee at Chattanooga
615 McCallie Ave, Chattanooga, TN 37403
Phone: 423-425-4017
Email: reetesh-ranjan@utc.edu
ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

**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-LESLE 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-LESLE 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:**


**External Conferences:**


Presentations at UTC:


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


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


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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
<tbody>
<tr>
<td>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:</td>
<td></td>
</tr>
<tr>
<td>• Constructing structural models of the N protein.</td>
<td></td>
</tr>
<tr>
<td>• Performing MD simulations to study structural and binding conformational dynamics.</td>
<td></td>
</tr>
<tr>
<td>• Determining the specificity and stability of the aptamer-N protein complex.</td>
<td></td>
</tr>
<tr>
<td>The outcomes of this project so far includes</td>
<td></td>
</tr>
<tr>
<td>• 2 submitted proposals (NIH &amp; NSF PI Danquah)</td>
<td></td>
</tr>
<tr>
<td>• 2 research manuscripts under review</td>
<td></td>
</tr>
<tr>
<td>• Support for 1 PhD student</td>
<td></td>
</tr>
</tbody>
</table>

![Fig. 2. Structure of SARS-COV-2 N protein showing the N terminal RBD.](image)

<table>
<thead>
<tr>
<th>RESULTS</th>
<th>OTHER INFO</th>
</tr>
</thead>
<tbody>
<tr>
<td>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 to other domains of the protein.</td>
<td></td>
</tr>
<tr>
<td>Structural modeling of the RBD of SARS-CoV-2 N protein showed that</td>
<td></td>
</tr>
<tr>
<td>• 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.</td>
<td></td>
</tr>
<tr>
<td>Budget and Schedule</td>
<td></td>
</tr>
<tr>
<td>Total Budget: $20,000</td>
<td></td>
</tr>
<tr>
<td>Actual Used: $20,000</td>
<td></td>
</tr>
<tr>
<td>Balance: $0</td>
<td></td>
</tr>
<tr>
<td>Total period of performance is 4 months.</td>
<td></td>
</tr>
<tr>
<td>Task 1: Months 1-5: Constructing structural models of the SARS-CoV-2 N protein.</td>
<td></td>
</tr>
<tr>
<td>Deliverables</td>
<td></td>
</tr>
<tr>
<td>• 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</td>
<td></td>
</tr>
<tr>
<td>• 2 submitted proposals (NIH &amp; NSF PI Danquah)</td>
<td></td>
</tr>
<tr>
<td>• 2 research manuscripts under review</td>
<td></td>
</tr>
</tbody>
</table>
• 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.

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

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)

**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.
**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](image)

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.

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**Budget and Schedule**

<table>
<thead>
<tr>
<th>Description</th>
<th>Amount</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Budget</td>
<td>$20,000</td>
</tr>
<tr>
<td>Actual Used</td>
<td>$20,000</td>
</tr>
<tr>
<td>Balance</td>
<td>$0</td>
</tr>
</tbody>
</table>

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

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

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.
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.
<table>
<thead>
<tr>
<th>PROJECT TITLE</th>
<th>Technology Area of Interest: Health and Biological Systems</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>TECHNICAL APPROACH</strong></td>
<td><strong>OUTCOMES</strong></td>
</tr>
<tr>
<td>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.</td>
<td>We accomplished the following:</td>
</tr>
<tr>
<td>Tasks included:</td>
<td></td>
</tr>
<tr>
<td>• Collect data social organization and life history dataset for artiodactyls</td>
<td>1. Data on artiodactyl group sizes collected for ~200 populations.</td>
</tr>
<tr>
<td>• Develop plan for mathematical modeling</td>
<td>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).</td>
</tr>
<tr>
<td>• Extract rainfall data from online data sources</td>
<td>3. Wang developed a mathematical model using data provided by Pope.</td>
</tr>
<tr>
<td>• Develop search tools based on machine learning</td>
<td>4. Azad Hossain and student extracted rainfall data for &gt;10 years from the online database (CRU). This project will be completed Summer 2021.</td>
</tr>
<tr>
<td></td>
<td>5. Suggs presented data on his machine learning project at a national meeting.</td>
</tr>
<tr>
<td><strong>RESULTS</strong></td>
<td><strong>OTHER INFO</strong></td>
</tr>
<tr>
<td>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.</td>
<td>Due to a change in personnel and the COVID-19 pandemic, the project has been extended until June 2022.</td>
</tr>
<tr>
<td><strong>Budget and Schedule</strong></td>
<td></td>
</tr>
<tr>
<td>Total Budget: $98,662.00</td>
<td></td>
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<tr>
<td>Actual Used: $67,528.33</td>
<td></td>
</tr>
<tr>
<td>Balance: $31,133.67</td>
<td></td>
</tr>
<tr>
<td>Total period of performance is 12 months.</td>
<td></td>
</tr>
<tr>
<td><strong>Deliverables</strong></td>
<td></td>
</tr>
<tr>
<td>• Quarterly reports describing progress and challenges</td>
<td></td>
</tr>
<tr>
<td>• Final report detailing results, financials, and future work</td>
<td></td>
</tr>
<tr>
<td>• Paper submitted to Journal of Mammalogy</td>
<td></td>
</tr>
<tr>
<td>• UTC Research Dialogues presentation</td>
<td></td>
</tr>
</tbody>
</table>
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.

<table>
<thead>
<tr>
<th>List of Objectives / Aims / Major Milestones Proposed</th>
<th>Cumulative Outcomes / Accomplishments</th>
</tr>
</thead>
<tbody>
<tr>
<td>Building an artiodactyl dataset</td>
<td>Added information on group size, moved species level information to populations, and added life history data from primary literature</td>
</tr>
<tr>
<td>Life history analysis</td>
<td>Compared data from primary literature to online database and conducted statistical analysis</td>
</tr>
<tr>
<td>Rainfall dataset</td>
<td>Used GPS locations from artiodactyl dataset, we are now extracting rainfall data (1900-present) from CRU dataset</td>
</tr>
<tr>
<td>NSF proposal</td>
<td>Submitted an NSF proposal in Summer 2020. The proposal built on aims of this project.</td>
</tr>
<tr>
<td>Connected CEACSE funded project to Hayes’ NSF IRES grant</td>
<td>A student working on a related project (mating systems) is collaborating with Schradin (France). The student is funded by Hayes’ NSF IRES program.</td>
</tr>
<tr>
<td>Build student capacity</td>
<td>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.</td>
</tr>
</tbody>
</table>
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.

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:**


**External Conferences:**


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:**


**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-Pl(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 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

<table>
<thead>
<tr>
<th>TECHNICAL APPROACH</th>
<th>OUTCOMES</th>
</tr>
</thead>
<tbody>
<tr>
<td>• List of tasks</td>
<td>The team has conducted a comprehensive literature review and identified similar work for potential knowledge transfer and to help with the work proposed herein.</td>
</tr>
<tr>
<td>1- Literature Review</td>
<td>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.</td>
</tr>
<tr>
<td>2- Equipment Purchase, installation, and configuration</td>
<td>The team is currently working on the development and integration process.</td>
</tr>
<tr>
<td>3- Developing an Integrated Heterogeneous Simulator</td>
<td></td>
</tr>
<tr>
<td>4- Developing a Behavioral Data Collection and Visualization Interface</td>
<td></td>
</tr>
<tr>
<td>5- Developing Use Case for SmartSim</td>
<td></td>
</tr>
<tr>
<td>6- Writing Final Report and Planning for Extramural Funding</td>
<td></td>
</tr>
</tbody>
</table>

## RESULTS

None yet.

## OTHER INFO

### 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
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 severely 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.