THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

Annual Report to the Tennessee Higher Education Commission: Fiscal Year 2019–2020

OCTOBER 15, 2020

Submitted by
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THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

SIMCENTER

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

CENTER OF EXCELLENCE

IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

MISSION STATEMENT

To establish, expand, and sustain a cohesive multidisciplinary effort in applied computational sciences through mentoring of students and faculty, seed funding in key thrust areas, and state-of-the-art research computing facilities.

VISION STATEMENT

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

EXECUTIVE SUMMARY

The University of Tennessee at Chattanooga's (UTC) Center of Excellence in Applied Computational Science and Engineering (CEACSE) continues its second decade of invigorating scientific inquiry, bolstering the learning environment, broadening participation, and establishing sustainable research pathways that benefit our institution, faculty and students, and the State of Tennessee. With our previous report for FY2020, CEACSE marked its 14th 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 FY2020 follows up our previous report with CEACSE's focused priority areas, highlights the ongoing strengths of its visionary leadership team, and notes greater impacts across a range of stakeholder groups. CEACSE comprises the indispensable factor that enables UTC to recruit, retain, and engage outstanding professors and equally outstanding students through research experiences for undergraduates up to and including PhD students.

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

Notable outcomes in FY2020 include these highlights:

- From CEACSE funds, we awarded eight core awards ($100,000), five Initiation/Opportunity Awards ($15,000), and two Lecture Series Grants ($2,500) in FY2020.
- We launched three new research thrusts: Digital Twins (led by Dr. Abi Arabshahi), Extreme Systems (led by Dr. Daniel Loveless), and Advanced Modeling & Simulation (led by Dr. Eleni Panagiotou).
- Dr. Don Reising, leader of the Environment research thrust, received $100,000 from the ORNL/UT/Launch Tennessee RevV! program for a project entitles "Safer Power Network" with Hayden Data Systems
- Drs. Anthony Skjellum and Craig Tanis, leaders of the High-Performance Computing & Algorithms research thrust, received $100,000 from the Sandia National Laboratories for continued studies of Exascale Computing.
- Dr. Anthony Skjellum received $60,000 from the Lawrence Livermore National Laboratory for Fault-Tolerant HPC Research.
- Dr. Anthony Skjellum received $32,000 in REU Supplement funding for existing awards.

- Dr. Farah Kandah, leader of the Cybersecurity & Cyber-physical Systems thrust, received $16,000 in REU Supplement funding for existing awards.
- Dr. Anthony Skjellum received a supplement of $103,537 to his award “SHF: Medium: Collaborative Research: Next-Generation Message Passing for Parallel Programming: Resiliency, Time-to-Solution, Performance-Portability, Scalability, and QoS.”
- Drs. Reetesh Ranjan and Abi Arabshahi submitted a proposal to the Department of Defense Investigator-Initiated Research Award competition, for a project related to computational modeling of human airways, especially to be used in treating respiratory infections that result from COVID-19.
- Drs. Reetesh Ranjan, Abi Arabshahi, Trevor Elliott, Henry Spratt, David Levine, Chuck Margraves, and Abdul Ofoli submitted a proposal to the Department of Defense Investigator-Initiated Research Award competition, for a project related to COVID-19 air filtration and sanitizing.
- With CEACSE funds, the SimCenter supported four projects related to COVID-19 research: Dr. Michael Danquah, Dr. Abi Arabshahi, Dr. Soubantika Palchoudhury, and Dr. Eleni Panagiotou. Their work is outlined in the next pages.
- Dr. Anthony Skjellum co-organized, with the University of Tennessee, an exhibitor booth at SC19, a collaboration that is likely to be annual.
- Dr. Anthony Skjellum co-led an Exascale MPI workshop at SC19 (The International Conference for High Performance Computing, Networking, Storage, and Analysis). Other organizers included Sandia National Lab, the EPCC (Edinburgh Parallel Computing Centre, a supercomputing center based at the University of Edinburgh), and the University of Alabama at Birmingham.
- Technical collaborations within the SimCenter led to the creation of the “Advanced Modeling & Simulation” and “Extreme Systems” thrusts in FY2020. The Aerospace and Defense thrust graduated from the SimCenter through its excellence in performing research and securing funding.
- Drs. Anthony Skjellum, Craig Tanis, and Abi Arabshahi received advance authorization to proceed on PSAAP-III funding from the Department of Energy. The 5-year, $4,000,000 award is led by the University of New Mexico.

Important technical advancements achieved in FY2020 include these highlights:

- Dr. Anthony Skjellum co-organized the First Workshop on Compiler-assisted Correctness Checking and Performance Optimization for HPC (C3PO’20), held virtually in June 2020. The workshop brought together researchers with a shared interest in applying compilation and source-to-source translation methodologies to enhance parallel programming, including explicit programming models such as MPI, OpenMP, and hybrid models.
- Drs. Loren Hayes and Craig Tanis collaborated on a predictive modeling project at the intersection of computer science and biology. They developed an automated search platform to obtain papers from the Google Scholar database to help researchers determine whether the stored papers are suitable for a given project. This work led to an NSF proposal to the Integrative Organismal Systems program.
- Drs. Jennifer Boyd and Craig Tanis used network analysis, a tool useful for analyzing connections between parts of a system, in an unconventional way to examine the integration of ecological and evolutionary research foci in studies of plant species rarity.

Dr. Boyd's empirical work focuses on the abilities of rare species to acclimate and adapt to environmental change, which involves both ecological and evolutionary processes, so this network analysis helps provide context for her work. This project involved a collaboration between UTC undergraduates Thomas Wiegand and Braley Gentry and former graduate student Zach McCoy; UTC faculty mentors with expertise in ecology (Dr. Jennifer Boyd), evolution (Dr. Hope Klug), and computational methodologies (Dr. Craig Tanis); and a mathematical biologist from the University of Oxford (Dr. Mike Bonsall).

- Drs. Daniel Loveless (leader of the Extreme Systems thrust) and Anthony Skjellum created a new FPGA testbed and updated the existing IBM Power9 testbed with new nodes.
- In FY2019, Dr. Farah Kandah was awarded $499,663 from the National Science Foundation for the project entitled "CC* Networking Infrastructure: Advancing High-speed Networking at UTC for Research and Education," to support 100Gbit/s networking to connect CEACSE computing and data resources with seven other campus R&D centers, enabling modeling and simulation work and accessibility across campus. Deployment of these resources began in FY2020.

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

This document constitutes the Annual Report for Fiscal Year 2020 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 FY2020 Awardees

The following faculty and staff were integral to the strategic direction of CEACSE during the 2019–2020 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. Shellie Acocello

Shellie Acocello serves as the Program Director of the Graduate Athletic Training Program at the University of Tennessee at Chattanooga. In her seventh year at the university, she focuses her research on identifying sensitive methods for diagnosing sport-related concussion and determining adequate readiness for return to sport following concussion. Previous research has included measurement of cerebral blood flow as well as pre- and post-injury screening including neuropsychological testing, simple and complex measures of visuomotor reaction time, and psychosocial consequences of injury.

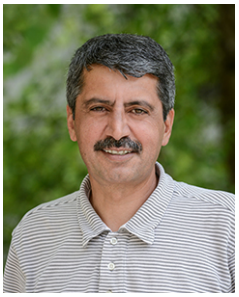
Co-Investigator: "The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"

Dr. Fernando Alda

Fernando Alda is an Assistant Professor in the Department of Biology, Geology and Environmental Science. He completed his undergraduate and graduate studies at the University of Navarra and the National Museum of Natural Science, in Spain, where he is originally from. He has carried out postdocs at the Smithsonian Tropical Research Institute in Panama, Tulane University, and Louisiana State University. In his research, he wants to understand how and why species originate and diverge from one another. Most of the time, he looks at the diversity of freshwater fishes to answer these questions. He uses molecular (genetic and genomic) and computational tools, together with data collected in the field and natural history collections, to reconstruct the evolutionary history of species and test hypotheses about their evolution. He is also interested in methodological questions such as best methods and data types to obtain accurate species trees.

Lead PI: "Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)"

Dr. Abdollah Arabshahi



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

Co-Investigator: "Polymer Entanglement"

Dr. Jejal Reddy Bathi

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

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

Dr. Ashley Manning-Berg

Ashley Manning-Berg received her PhD and MS from the University of Tennessee Knoxville. Her research involves using chemical sedimentary rocks to investigate the geochemical composition of Earth's surface environments and the effects of early diagenesis in these systems. She is also interested in early life on Earth and the interaction between that life and Earth's early environments. Most of her research has focused on the Precambrian, and the geochemical conditions of marginal marine environments and early Earth. Such geologic settings aid in our understanding of early life on Earth, how that life was preserved in the rock record, and provide analogs for potential extraterrestrial microbial life.

Lead PI: "Modeling of microbial mat decay and implications for the early Earth fossil record"

Dr. Stephanie DeVries

Stephanie DeVries is a hydrogeologist and aqueous geochemist conducting research in groundwater modeling and contaminant transport. She is currently working on a nitrate prediction tool that uses input from groundwater flow models, USDA crop data, and climate data to estimate the concentration of nitrate in a high-capacity pumping well. She is also working with the Tennessee Department of Environment and Conservation to geolocate residential septic permits through a Service Learning Program at UTC. The data product will have significant value for investigating impacts of septic density or placement on surface water quality. Finally, she is mentoring several student research projects that use analytical and geospatial tools to examine water quality issues related to foundry waste, microplastics, and septic waste systems.

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

Mr. Chris Dowell

Chris Dowell has a 20+ year IT history working for companies such as Lexmark, IBM and Oracle. He recently moved to Chattanooga from Bozeman, MT. Chris lends his expertise to all SimCenter students and projects as one of the primary High-Performance Computing System Administrators in the Multidisciplinary Research Building. His work is focused on helping users orient to a clustered computing environment and on solving their technical issues while improving and maintaining the existing computing infrastructure.

Co-Investigator: "Polymer Entanglement"

Dr. David Giles

David Giles is an Associate Professor for Biology, Geology and Environmental Science. He received a BA (2001) in Biology from Maryville College and a PhD (2008) in Biomedical Sciences with a concentration in Microbiology from East Tennessee State University. His research and involves assessing impacts of exogenous fatty acids on membrane composition and virulence of Gram-negative bacteria, with four publications on the topic since 2017. Dr. Giles uses microbiology, genetics, and biochemistry to investigate bacteria of medical importance in response to environmental and host-specific conditions.

Co-Investigator: "The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence"

Dr. Bradley Harris

Bradley Harris is an Assistant Professor in the Department of Civil and Chemical Engineering at UTC. He received his PhD (2014) in Chemical and Biomolecular Engineering at UTK. He is the Chemical Hygiene Officer for CECS and the faculty advisor for the UTC student chapter of the American Institute of Chemical Engineers (AIChE). His research interests are in bioengineering, specifically the application of chemical engineering principles to biological problems. He is also passionate about undergraduate research and seeks to maintain a laboratory offering opportunities for chemical engineering students interested in bio-related research. His areas of expertise are biochemistry and cellular and molecular biology, with applications in renewable energy and disease pathogenesis. In his current research, Dr. Harris is studying how bacterial pathogens sense and respond to their environment in an effort to improve disease control strategies.

Dr. Harris is also interested in engaging local community college students in chemical engineering through cyber-physical systems (CPS). Dr. Harris is actively working to bring online lab stations involving unit operations such as absorption, distillation, heat transfer, fluid flow, and reaction kinetics through the use of Internet of Things. This project is funded by a NSF RET grant (Award #1953645), and it is part of a greater effort by UTC and the City of Chattanooga to advance technologies for smart cities by using CPS to manage assets and resources efficiently. Please refer to Dr. Harris' biosketch in Appendix A for more information.

Lead PI: "The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence"

Dr. Loren Hayes

Loren Hayes is an Associate Professor in Biology, Geology and Environmental Science. He received his BS in Biology from Bates College, MS in Zoology from Michigan State University, and PhD from Miami University. His research interests include the fitness consequences of communal living and the drivers of social evolution in mammals. He has 50 publications in a range of internationally reputable journals, including *Animal Behavior*, *Behavioral Ecology, Biology Letters, Ethology, Journal of Mammalogy, Trends in Ecology and Evolution,* and *Proceedings of the Royal Society B*. He has published numerous book chapters and co-edited a book on the sociality of caviomorph rodents. He regularly presents his research at international conferences and is co-host of a remote, international seminar series on social evolution. He has generated nearly $1 million in research funding, mostly from NSF.

Lead PI: "Using Computational Approaches to Enhance Comparative Studies of Social Evolution"

Dr. Jennifer Hogg

Jenny Hogg attended Troy University for her Bachelor's in Athletic Training. She then attended the University of Alabama where she was a graduate assistant athletic trainer for the men's and women's varsity tennis teams. For 5 years she was the athletic trainer for Gulf Coast State College athletics in Panama City, FL, before she returned to grad school, completed her PhD in Applied Neuromechanics at the University of North Carolina Greensboro in 2018. She is currently in her 4th year at UTC. My primary interests are the identification of risky lower extremity biomechanics, specifically in relation to anterior cruciate ligament injury. Secondarily, upon identification of such risky movement patterns, my recent work has incorporated novel motor learning techniques and technological advances to retrain functional movement for prevention of primary and secondary ACL injuries in both male and female cohorts.

Lead PI: "The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"

Dr. Azad Hossain

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

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

Dr. Hamdy Ibrahim

Hamdy Ibrahim is an Assistant Professor in the Mechanical Engineering Department at the University of Tennessee at Chattanooga. Before joining UTC, he worked as a postdoctoral fellow in the dynamics and smart systems lab (DSSL) at the University of Toledo, Ohio. He also worked as a Chief Research Officer for the start-up company Thermomorph, LLC aims to develop Nitinol-based biomedical devices. Dr. Ibrahim completed his PhD in Mechanical Engineering from the University of Toledo in August 2017. He also completed his MSc in May 2012 after obtaining a BSc Hons Degree in May 2008, both in Mechanical Engineering, from Cairo University. Dr. Ibrahim's research findings on biomaterials have resulted in 2 patent applications and over 20 peer-reviewed journal and conference publications. His research interests are focused on

biodegradable metals, biocomposites, shape memory alloys, additive manufacturing, surface treatments, and corrosion behavior of biomaterials.

Lead PI: "Corrosion Modeling of Magnesium-Based Fixation Hardware For Mandibular Reconstruction Surgeries"

Dr. Farah Kandah

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

Lead PI: "Decentralized and Scalable Trust Management Approach Via Blockchain for Connected Vehicles in Smart Cities"

Dr. Francesca Leasi

Francesca Leasi is an Assistant Professor in the Department of Biology, Geology, and Environmental Science. She received her MS and Ph.D. degrees from the University of Modena and Reggio Emilia, Italy (2002 and 2007) in Biology Ecology and Evolutionary Biology. Dr. Leasi's research interests include biodiversity, macroecology, and patterns of diversity and distribution, mostly using as a test case microscopic invertebrates. To explore such topics, she uses an integrated approach of morphology-based and DNA taxonomy, high-throughput sequencing, and computational biology. Microinvertebrates are largely unknown, yet they are important contributors to ecosystem functioning and food web interactions. Dr. Leasi has been supported by CEACSE to explore the microinvertebrates from Hamilton County and understand how their biodiversity is affected by anthropogenic activities. She has thus far published 40 peer-reviewed articles, 2 invited book chapters, and presented in over 50 conferences, whereas the first report on the biodiversity of microscopic invertebrates from Hamilton County is currently in preparation and will be soon submitted to a peer-reviewed journal.

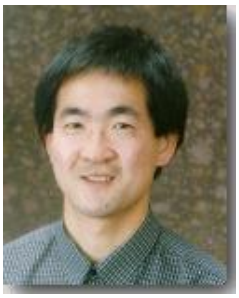
Lead PI: "Simulating bio-environmental interactions using –omics approaches"

Dr. John P. Lee

John P. Lee obtained a B.S. in chemistry from the University of Tennessee at Chattanooga (UTC) under the direction of Prof. Gregory J. Grant. After completing his Ph.D. at North Carolina State University with Prof. T. Brent Gunnoe he spent two years as a research chemist at Eastman Chemical Company. He then accepted a teaching-research postdoctoral position under the direction of Grant at UTC, and subsequently joined the faculty at UTC in 2012. Research in the Lee group is undergraduate-focused with interest in the development of new inorganic and organometallic complexes for potential use in homogeneous catalysis.

Co-Investigator: "Alkynyl Tetrafluoro-Pyridyl Ligands: Computational Studies, Synthesis, and Characterization"

Dr. Yu Liang



Yu Liang is a Professor in the Department of Computer Science and Engineering of UTC. His funded research covers machine learning, big-data and cloud computing, modeling and simulation, high-performance scientific and engineering computing, numerical linear algebra, data-driven medical instruments design, and computational mechanics. His research has appeared in various journals; book or book chapters; and refereed conference, workshop, and symposium proceedings. Currently, Dr. Liang has five federal-funded projects. Dr. Liang serves on the International Journal of Security Technology for Smart Device (IJSTSD), Journal of Mathematical Research and Applications (JMRA), and Current Advances in Mathematics (CAM) as an editorial board member.

Co-Investigator: "The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"

Dr. Mohammad Mahtabi

Mohammad Mahtabi received his PhD in Mechanical Engineering from Mississippi State University and was a post-doctoral researcher for about a year at The University of Toledo, before joining the Mechanical Engineering Department at UTC. Dr. Mahtabi holds a bachelor's degree from The University of Tehran and a master's degree from Iran University of Science and Technology. He has also worked for about seven years in the industry as a structural engineer. Dr. Mahtabi's research area includes experimental and computational aspects of additive manufacturing (a.k.a. 3D printing), fatigue and fracture mechanics, mechanical behavior of materials and shape memory alloys.

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

Dr. 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: "Polymer Entanglement"

Dr. Jared Pienkos

Jared Pienkos is an Assistant Professor for the Department of Chemistry and Physics. He received a BA (2009) in Chemistry/Math (double major) from Hamilton College. He then received his PhD from the University of Virginia (2014), working under Dr. Walter D. Harman where he developed synthetic methodology utilizing dearomatization reagents. Following graduate school, Dr. Pienkos completed a postdoctoral position at Furman University, working with Dr. Paul S. Wagenknecht to investigate the metal-to-metal charge transfer in Fe(II)/Ti(IV) compounds. Dr. Pienkos has authored 15 papers in peer-reviewed journals, including *Journal of the American Chemical Society*, *Inorganic Chemistry*, *Organometallics*, and *Dalton Transactions*. He currently has a research group of seven undergraduates and one high school student. Dr. Pienkos investigates transition metal alkynyl compounds with the aim of generating new catalysts and molecular devices (e.g., organic light emitting diodes). He his research students presented results of this work at the regional chemistry meeting, SERMACS.

Lead PI: "Alkynyl Tetrafluoro-Pyridyl Ligands: Computational Studies, Synthesis, and Characterization"

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.

Lead PI: "A Multi-Fidelity Computational Modeling Strategy for Large-Eddy Simulation of Turbulent Combustion"

Dr. Mina Sartipi

Mina Sartipi is the Founding Director of the Center for Urban Informatics and Progress (CUIP) and is also a Guerry Professor in the Computer Science and Engineering Department, where she leads the Smart Communications and Analysis Lab (SCAL). She received her BS in Electrical Engineering from Sharif University of Technology, Tehran, Iran, in 2001 and her MS and PhD degrees in Electrical and Computer Engineering from Georgia Tech in 2003 and 2006, respectively. She is a member of technical program committee for several workshops and conferences on topics related to AI and smart city operations. She was named 2019 Chattanooga Influencer by the Edge, Chattanooga's Business Magazine, for her role in Smart City research and collaboration with city, county, and industry partners. She is recipient of several awards including 2016 UT-Chattanooga Outstanding Faculty Research and Creative Achievement award, UC Foundation Professorship, and 2020 Smart 50 awards in Digital Transformation at the Smart Cities Connect (in collaboration with CHA and EPB). She has published over 50 papers related to data science, wireless communications, connected vehicles, and data integration. She has delivered several keynotes and presentations including US Congressional Caucus on Smart Cities, live demo of connected vehicle project at the Smart City Connect, and National Transportation Training Directors. Dr. Sartipi has been an IEEE senior member since 2016. She is a member of the Board of Directors for the Enterprise Center, Chattanooga, TN, Variable, Inc., Thrive Regional Partnership, and Mohuman. Dr. Sartipi's research interests are in the area of wireless communications and data analysis for smart city applications including mobility, health, and energy. Her research is supported by NIH, NSF, DOE, State of TN, foundations, and industry.

Co-Investigator: "Decentralized and Scalable Trust Management Approach Via Blockchain For Connected Vehicles in Smart Cities."

Dr. Mark Schorr

Mark Schorr received his BS in Zoology from Southeastern Louisiana University, his MS in Zoology from Mississippi State University, and his PhD in Forest Resources (Fisheries Management) from Mississippi State University. His primary research interest is stream fish ecology, with an emphasis on water pollution issues and population/community ecology. Graduate and undergraduate students working in his laboratory have conducted research to address the following problems: (1) influence of coal mine drainage on stream water chemistry, habitat, and aquatic macrofauna (macroinvertebrates, fishes, salamanders) in the Cumberland Plateau; (2) landscape-stream

relationships that involve watershed land use, riparian buffers, limnological parameters, and macrofaunal assemblages in Ridge and Valley catchments; (3) localized effects of road culverts on instream habitat and fish assemblages in Blue Ridge catchments; (4) lotic macrofaunal responses to stream restoration projects (artificial pools/riffles, constructed channels); and (5) historical and contemporary patterns in the distribution and abundance of the introduced redbreast sunfish (*Lepomis auritus*) and native congeneric sunfishes (*Lepomis* spp.; Centrarchidae) in reservoirs in the Tennessee River drainage.

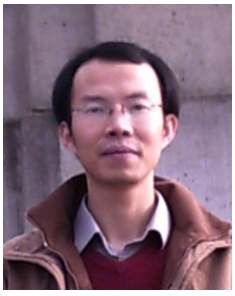
Co-Investigator: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"

Dr. Craig Tanis

Craig Tanis is an Assistant Professor in Department of Computer Science and Engineering. He received his BSE in Computer Engineering and MS in Computer Science from Tulane University in 1997 and 1998, respectively. He received his PhD in Computational Engineering from UTC in 2013. Dr. Tanis researches the use of programming language techniques in HPC, helping application scientists develop correct codes without compromising computational efficiency. His expertise lies in HPC, programming languages, and interactive multimedia.

Co-Investigator: "Using Computational Approaches to Enhance Comparative Studies of Social Evolution"

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: "Polymer Entanglement"

Dr. Gary Wilkerson

Gary Wilkerson is a tenured professor at the University of Tennessee at Chattanooga, where he has taught in the Graduate Athletic Training Education Program since 1999. Over the past five years, his research publications have been cited by more than 850 authors. He was among the first scholars to receive the designation of National Athletic Trainers' Association Fellow after the honor was created in 2008, he was inducted to the NATA Hall of Fame in 2016, and he was awarded the NATA Foundation Medal for Distinguished Research in 2019. His recent research has been focused on development of methods for clinical identification of subtle

perceptual-motor performance deficiencies that elevate risk for concussion and musculoskeletal injury.

Co-Investigator: “The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation”

Dr. Dalei Wu

Dalei Wu is a UC Foundation Associate Professor in the Department of Computer Science and Engineering at the University of Tennessee at Chattanooga. His research interest includes sequential decision theory, data-driven intelligent systems, sensor networking, and mobile computing. He has published research papers in a variety of prestigious journals, such as *ACM Transactions on Modeling and Computer Simulation*, *IEEE Internet of Things Journal*, *IEEE Transactions on Industrial Informatics*, *IEEE Transactions on Automatic Control*, *IEEE Transactions on Circuits and Systems for Video Technology*, *IEEE Transactions on Wireless Communications*, *IEEE Journal on Selected Areas in Communications (JSAC)*, *IEEE Transactions on Multimedia*, and *IEEE Transactions on Communications*. His research has been supported by NSF and the State of Tennessee. He is an Associate Editor of IEEE Internet of Things Journal and IEEE Access.

Co-Investigator: “The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation”

Dr. Sungwoo Yang

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

Lead PI: “Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling”

Dr. Wang-Yong Yang

Wang-Yong Yang is an Assistant Professor of Chemistry at the University of Tennessee-Chattanooga. He earned his Bachelors and Masters of Science in Chemistry at Pusan National University, Korea, in 1996 and 1998, respectively. Following this, he joined Dong-Wha Pharmaceutical Ind. Co., Korea as a research scientist. For 6 years in the company, he focused on two projects: 1. *Development of Non-nucleoside HBV & HCV Inhibitors,* 2. *Development of Potent Quinolone Class Antibiotics*. He then moved to USA and received his PhD in Organic Chemistry from Florida State University, Tallahassee in 2011, working with Dr. Igor Alabugin. His dissertation titled *Design of pH-Controlled Light-Activated Reagents for Efficient Cleavage of Double-Stranded DNA and Cancer Phototherapy.* After completing his PhD, Yang started his postdoctral fellowship in the Scripps Research Institute in Jupiter, FL, under supervision of Dr. Matthew Disney. During that time, he developed *Small Molecules Targeting Toxic RNAs related to Human Neurodegenerative Diseases such as Fragile X-associated tremor/ataxia syndrome (FAXTAS) and spinocerebellar ataxia-10 (SCA10)*. In 2018, Yang accepted an Assistant Professor position at University of Tennessee-Chattanooga. His current research interests include "*switchable*" bioactive organic molecules controlled by an external stimulus (e.g, pH, light). He is also interested in studying structural and electronic properties of organic molecules that determine chemical activities of the molecules.

Co-Investigator: "Polymer Entanglement" & Alkynyl Tetrafluoro-Pyridyl Ligands: Computational Studies, Synthesis, and Characterization"

FY2020 STUDENTS

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

Students Impacted:

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

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

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

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

Project Title: Polymer Entanglement
Lead PI: Eleni Panagiotou

Students Impacted:

Evan Gildernew: Participated in research and gave poster presentation, graduate student, MS Chemical Engineering

Peter Zeglen: Participated in research, graduated Bachelor's in Mathematics

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

Matthew Phanner: Participating in research, Bachelor's in Chemistry

Justin Pease: Participating in research, Bachelor's in Chemistry

Project Title: “Corrosion Modeling Of Magnesium-Based Fixation Hardware For Mandibular Reconstruction Surgeries”

Lead PI: Mohammad Mahtabi

Students Impacted:

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

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

Alexander Joplin: Undergraduate student. He was partially funded in this project during Spring and Summer 2020.

Clay Jones: He was partially funded in this project during Spring 2020.

Project Title: “Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling”

Lead PI: Sungwoo Yang

Students Impacted:

Evan Gildernew: 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 is now considering pursuing a Ph.D. program at UTC.

Emily Chase: (2020 graduated) was an undergraduate student who has been working on the synthesis of 3dCN for a year. She found interests in research and joined Northwestern University to purse her Ph.D. in Chemical Engineering.

Jasper Emerton: undergraduate student and eager to learn about Python and FeniCS.

Alex Rutter: undergraduate student and eager to learn about Python and FeniCS.

Erik Loredo: undergraduate student and eager to learn about Python and FeniCS.

John Roberts: undergraduate student and eager to learn about Python and FeniCS.

Project Title: “Decentralized and scalable trust management approach via blockchain for connected vehicles in smart cities.”

Lead PI: Farah Kandah

Students Impacted:

Brennan Huber: M. Sc Computer Science: Cyber security. During the period of performance, Mr. Huber acquired a good amount of experience into coding and developing and evaluating the system.

Amani Altarawneh: PhD Computational Science: Computer Science. Ms. Altarawneh acquired a great experience related to designing Blockchain approaches that is applicable to IoT systems setup.

Sai Madury: PhD Computational Science: Computer Science. Mr. Madury acquired a great experience in programming and dealing with OpenStack clustering to develop and simulate a Blockchain based communication system to evaluate the applicability of Blockchian in dynamic system setups.

Jacob Coleman: M.Sc. Computer Science. Mr. Coleman acquired a great experience in machine learning and how it related to different applications in smart cities setups including trust management in IoT systems (specifically Ocean of Things).

Jonathan Hunter: M.Sc Computer Science. Mr. Hunter investigated the applicability of Blockchain in IoT systems which provided him with a great understanding of how Blockchain can assist in providing a tamper proof, global view of the data shared among the system's entities. Also, he acquired good experience in coding and developing using Raspberry Pis.

Sree: M.Sc. Computer Science. Ms. Sree implemented a computer vision (CV) algorithm on edge and was introduced to different CV algorithms.

Project Title: "Alkynyl Tetrafluoro-Pyridyl Ligands: Computational Studies, Synthesis, and Characterization"
Lead PI: Jared A. Pienkos

Students Impacted:

Hailey Beaver: Biology major (Class of 2022). She plans on attending medical school.

Sarah McDarmont: Chemistry major (Class of 2021). She plans on attending graduate school.

Sophia Neglia: Chemistry major (Class of 2021). She plans on attending graduate school.

Logan Jaques: Chemistry major (Class of 2021). He plans on attending graduate school or getting a job at a chemical company.

Anastasia McConkey: A chemistry major (Class of 2020). Received a job at New Blooms Laboratory.

Tiffany Truong: a chemistry major (Class of 2022). She plans on attending graduate school.

Zach Moser: Chemistry major (Class of 2020). Received a job at Aegis.

Jasmine Suggs: Chemistry major (Class of 2020). Looking for an industrial chemistry job.

Brandon Nessell: Chemistry major (Class of 2022). He plans on attending graduate school.

Project Title: "The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence"

Lead PI: Bradley Harris

Students Impacted:

Konner Glass: Seeking B.S. ChE. Gained valuable experience in experimental design and execution, and presented research at local conferences.

Devin Martin: Seeking B.S. ChE. Gained valuable experience in experimental design and execution, as well as literature review and manuscript preparation.

Diane Madeksho: Seeking B.S.Chemistry. Gained valuable experience in literature review and manuscript preparation.

Dalton Strike: B.S. ChE Spring 2020. Gained valuable experience in experimental design and execution, functioned as research team lead through training and mentoring of fellow ugrad students, and presented research at numerous local, regional, and national conferences. This research was also the focus of his DHON thesis.

Andrew Turgeson: Seeking Ph.D. in Computational Engineering. Gained valuable experience in computational modeling and structural analysis of biomacromolecules, as well as literature review and manuscript preparation.

Project Title: "The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"

Lead PI: Jennifer Hogg

Students Impacted:

Ashley Williams: Graduate student in Athletic Training

Samantha Kendall: Graduate student in Athletic Training

Colton Jenkins: Graduate student in Athletic Training

Meredith Davis: Graduate student in Athletic Training

Justin Ramos: Graduate student in Athletic Training

Abigail Rucker: Graduate student in Athletic Training

Griffin Miller: Computer Science & Engineering student

Zoe Zimmerman: Computer Science & Engineering student

Nicholas Milburn: Computer Science & Engineering student

Project Title: "Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)"
Lead PI: Fernando Alda

Students Impacted:

Taya de Blonk: A senior at UTC and will be graduating in the Fall of 2020. She has been working in the collection and dissection of tissues for RNA extraction and on the development of an automated bioinformatic pipeline for the assembly, annotation and analysis of genomic data. During the Summer of 2020 she is involved in the iCompBio REU program.

Tiffany Harvey: A transfer student from Chattanooga State. Tiffany has been working on the analysis of genomic data and the comparison of genes involved in the generation of electric signals. She was awarded a grant from the Honors School to work on her project during the Spring of 2020 and she will continue working on this project as part of her Departmental Honors Thesis during the academic year 2020-2021. Tiffany has also been a recipient of the Craig Scholarship awarded by the Department of Biology, Geology and Environmental Science for her research accomplishments during the past year.

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

Students Impacted:

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

William (Garrett) Hooten: Computer Science (’22). Programmed a stand-alone program that calculates the concentration of a contaminant well water as a function of land use using input data from USDA CropScape and a 3D groundwater flow model. Student gained valuable experience programming a practical application and will be featured as 2nd author on resulting publications. The student is also encouraged to present his work in the 2021 Research Dialogue

Project Title: “Using Computational Approaches to Enhance Comparative Studies of Social Evolution”
Lead PI: Loren Hayes

Students Impacted:

Evan Suggs: (Engineering and Computer Science, graduated May 2020) Evan worked as an hourly researcher on the project. He developed an automated search tool and worked on a senior thesis project on machine learning. His graduate work will be supported by Hayes and Tanis’ full CEACSE award.

Ashley Carpenter: (BGE, graduated May 2020) Ashley worked as an hourly researcher on the project. She conducted a validation study of the automated search tool for three taxonomic groups, showing that the method was effective at reducing effort. She also collected social organization data on the lagomorphs (rabbits, hares, pikas) and helped train French students using the search tool.

Harold Hansen: (Engineering and Computer Science, graduated in 2020) developed a website template for our project to partially fulfill the requirements for CPSC 4910.

Carter Hill: (Engineering and Computer Science, graduated in 2020) developed a website template for our project to partially fulfill the requirements for CPSC 4910.

Parshwa Patel: (Engineering and Computer Science, graduated in 2020) developed a website template for our project to partially fulfill the requirements for CPSC 4910.

Bowen Wexler: (Engineering and Computer Science, graduated in 2020) developed a website template for our project to partially fulfill the requirements for CPSC 4910.

Project Title: “A Multi-Fidelity Computational Modeling Strategy for Large-Eddy Simulation of Turbulent Combustion”

Lead PI: Reteesh Ranjan

Students Impacted:

Ashwyn Sam: He was first trained to use visualization software tools such as Paraview and Tecplot and Python for data analysis. Afterward, he learned to initialize isotropic turbulence using an in-house software referred to as TurbInit. Afterward, he was trained to solve laminar premixed flame configuration using Cantera. He set up and analyzed the turbulent premixed flame problem in physical and spectral space using Python-based tools. Also, he learned to conduct high-fidelity

fundamental turbulent combustion simulations using high-performance computing (HPC) resources at SimCenter and assessed the performance of OpenFOAM software for simulation of reacting and non-reacting flows. Finally, he was mentored on the essence of collaborative research and technical presentation and reporting skills.

Brennan Troxel: He was also initially trained for different software and computational tools such as Paraview, Pointwise, Python, etc. Afterward, he focused on the generation of computational mesh for LES of the established VOLVO combustor. In parallel, he learned the OpenFOAM software. After going through several tutorials, he set up the VOLVO case from scratch by following a published research article. He also got trained on the use of HPC resources at SimCenter and to perform scaling analysis for parallel computing. He ran the no-reacting flow within the VOLVO rig and documented all his findings in the form of weekly research presentations and mid-year and final reports.

Project Title: "Simulating bio-environmental interactions using –omics approaches"

Lead PI: Francesca Leasi

Students Impacted:

Preyanka Dey: MA Civil Engineering. She has been completely supported by CEACSE grant. Next year, she will be supported by Dr. Hope Klug and continue working on the watershed model.

Adrianna Hodges: MA Environmental Science. She was partially supported by CEACSE as she obtained a Teaching Assistantship from the BGES Department. Unfortunately, the collaboration did not work out and she stopped being supported a few months into the project. The carryover will be used to support undergraduates in biology, who will continue obtaining data.

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.

FY2020 has been another year of growth and enhancement for CEACSE. The leadership team is now comprised of 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 three years as of the date of this report, and he plans to grow and support work consonant with the original proposal to THEC for CEACSE. Continued emphasis on modeling and simulation in CSE, HPC/HPT, and data science ground the strategy of advancing and diversifying the participation of UTC faculty and students in CEACSE projects in FY2020 and beyond.

The FY2020 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).

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

We have also created three new thrusts: Digital Twins, Advanced Modeling & Simulation, and Extreme Systems. Digital Twins was active for the FY2020 CEACSE competition; the other two were formed afterward and are available as a proposal emphasis area beginning in FY2021. The Digital Twins thrust It provides a means to encapsulate R&D in modeling and simulation together with data fusion, analytics, and machine learning. This area of scientific and engineering pursuit is expected to be the key means by which modeling and simulation is delivered in real-time, for training, and for engineering analyses in many fields over the next two decades and beyond. This effort launches in complement to a new NSF award that will support workshops at UTC and Tennessee Technological University on the pedagogy of Digital Twins, with the goal of workforce development for this class of applied modeling and simulation workforce.

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:

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

These application focus areas were selected based on three important criteria:

- The presence of significant scientific and technical challenges for which there was interest, expertise, and the potential to excel at UTC;
- Clear alignment with educational and workforce development missions of UTC; and
- Opportunities to establish extramural R&D funding that can be realized by UTC researchers in strategic partnerships with collaborators at other institutions.

CEACSE proposals that fit these focus areas are reviewed for technical merit and strategic alignment, including scrutiny of a plan to develop extramural funding. Beginning in FY2019, further important advances in proposal content, process, selection, and peer review were applied across the CEACSE program. All CEACSE proposals 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 FY2020 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 FY2020 Projects

In FY2020, the core CEACSE competition awarded new seed funding to support the research activities of 22 faculty members for eight new projects from various disciplines across computational science and engineering. From a total of 26 proposals, these eight were selected for their potential to continue CEACSE efforts to broaden the scope of research through increased participation of additional faculty, graduate students, and undergraduate students. Faculty Initiation and Opportunity Awards included four faculty members on five new projects.

The funded projects key to the seven CEACSE/SimCenter priority areas active in FY2020: Aerospace & Defense, Cybersecurity & Cyber-physical Systems, Digital Twins, Energy & the Environment, Health & Biological Systems, High-Performance Computing & Algorithms, and Smart Cities & Urban Dynamics (in collaboration with UTC's Center for Urban Informatics & Progress (CUIP)). Not all thrusts are represented in these awards, but certain projects have elements that cross-cut multiple areas, such as Smart Cities & Urban Dynamics plus Energy & the Environment.

Appendix B provides the full PI-submitted reporting on each of the grants, including detailed final reports articulating the accomplishments, outcomes, and impacts for each award.

Core Competition

Project Title: Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling
Lead PI: Sungwoo Yang
Co-PI(s): N/A

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

Project Title: Alkynyl tetrafluoro-pyridyl ligands: computational studies, synthesis, and characterization
Lead PI: Jared Pienkos
Co-PI(s): Wang-Yong Yang, John Lee

Summary: Alkynyl compounds can be used to tune the absorption and emission properties of their corresponding transition metal complexes. Herein, we will describe the computational characterization and the synthesis of electron deficient alkynyl tetrafluoro-pyridyl ligands. Iridium, cobalt, and chromium alkynyl tetrafluoro-pyridyl metal ligand interactions will be modeled using a

variety of basis sets and functionals supported by the Gaussian/WebMO interface. Concurrent with these computational studies, representative iridium, cobalt, and chromium compounds will be synthesized. Following their synthesis and characterization, modulation of electrochemical and emissive properties will be performed by exploiting secondary binding sites. All of these interactions will be computationally modeled with the Gaussian/WebMO interface using resources within the SimCenter. Computational tools used in this project will also be implemented for educational outreach activities within the community.

Project Title: A study on the local and global effects of polymer entanglement in material properties and biological functions
Lead PI: Eleni Panagiotou
Co-PI(s): Jin Wang, Wang-Yong Yang, Abi Arabshahi

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

Project Title: Simulating bio-environmental interactions using –omics approaches
Lead PI: Francesca Leasi
Co-PI(s): Hong Qin, Jejal Bathi, Lani Gao

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

Project Title: Decentralized and Scalable Trust Management Approach via Blockchain for Connected Vehicles in Smart Cities
Lead PI: Farah Kandah
Co-PI(s): Mina Sartipi

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

Project Title: Corrosion modeling of magnesium-based fixation hardware for mandibular reconstruction surgeries
Lead PI: Hamdy Ibrahim
Co-PI(s): Mohammad Mahtabi

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

Project Title: The Use of Augmented Reality–Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation
Lead PI: Jenny Hogg
Co-PI(s): Shellie Acocello, Yu Liang, Gary Wilkerson, Dalei Wu

Summary: Ways in which the neuromuscular system can be leveraged to prevent both initial musculoskeletal and concussive injury and re-injury has been a key area of focus in the literature due to poor injury outcomes. Recent advances in scientific thought suggest that the central nervous system and neurocognition play a greater role in peripheral neuromuscular control than was previously assumed, which presents an opportunity for the development of injury

management programs. Because the brain is highly plastic and therefore trainable, research in this area will allow clinicians to take advantage of the brain's modifiable characteristics and devise rehabilitation strategies to improve both lower extremity injury outcomes and post-concussion management. The use of augmented reality–delivered, real-time feedback may serve to improve biomechanical and cognitive outcomes. The current proposal aims to fill that gap by determining the efficacy of using augmented reality to deliver movement feedback and the effect of the delivered feedback on neuromuscular activation, movement kinematics, and cognitive flexibility. Doing so will allow future studies to use the identified parameters to ultimately develop effective injury reduction and management programs.

Project Title: The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence
Lead PI: Brad Harris
Co-PI(s): Davy Giles

Summary: Bacterial pathogens are increasingly developing resistance to conventional antibiotics and represent a mounting threat to public health worldwide. This trend is due in part to the ability of these microorganisms to sense and adapt to their environment through endogenous membrane remodeling strategies. However, the ability of bacteria to adapt their membranes through uptake and assimilation of exogenous fatty acids remains largely unexplored. This project aims to quantify the extent to which exogenous fatty acids contribute to bacterial survival and persistence and to determine the molecular mechanisms by which fatty acid assimilation impacts membrane behavior. Uncovering this information will vertically advance our understanding of how fatty acids may serve as vital molecules that guide bacterial environmental adaptation and pathogen success. This research could also lead to the development of novel preventatives and therapeutics for antibiotic-resistant infections. Overall, the proposed project will contribute to capacity building and strategic excellence in computational science at UTC and potentially improve public health at large.

Project Title: Models of speciation based on the evolution of electric communication in weakly electric fishes
Lead PI: Fernando Alda
Co-PI(s): N/A

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

Project Title: A simplified subsurface characterization for local-scale groundwater flow models in unconfined sand and gravel aquifers
Lead PI: Stephanie DeVries
Co-PI(s): N/A

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

Project Title: Using computational approaches to enhance comparative studies of social evolution
Lead PI: Loren Hayes
Co-PI(s): N/A

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

Project Title: Modeling of microbial mat decay and implications for the early Earth fossil record
Lead PI: Ashley Manning-Berg
Co-Pi(s): N/A

Summary: Microbial mats are organic sedimentary structures that represent Earth's earliest ecosystems. Evidence for ancient microbial life can be found in 3.5 billion-year-old rocks, and in most cases, evidence is based solely on the morphology of the fossil. Many of the best fossils are preserved in microcrystalline silica, which would have required rapid silica precipitation early in the rock forming process before the microorganisms were significantly altered by decomposition. Taphonomic laboratory studies grow monocultures of cyanobacteria that are analogous to the cyanobacteria found in the fossil record and monitor changes to the morphologies of the organisms as they decompose. However, the effects of decomposition on microbial mat

preservation are unknown because growing microbial mats in a lab is difficult and time consuming. The proposed research will model microbial mat decay over time and use that model to predict the range of microfossil morphologies that would be observed in the rock record. Biomass accumulation within a mat will be calculated using a previously developed model and used in decomposition models to establish a relationship between biomass and time. The quality of microbial preservation can then be predicted based on the amount of time the mat was exposed to decomposition.

Project Title: A multi-fidelity computational modeling strategy for large-eddy simulation of turbulent combustion
Lead PI: Reetesh Ranjan
Co-Pi(s): N/A

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

Distinguished Lecture Series Grants

Requesting Faculty: Aniekan Ebiefung
Invited Speaker: Dr. Joaquim Judice, University of Coimbra, Aposentado, Portugal
Lecture Title: Complementarity Problems

Summary of Qualifications:
Professor Judice is an accomplished researcher in complementarity problems (CP). He has developed and implemented block pivoting algorithms for the LCP on many real life applications and found that are very efficient in dealing with large scale problems. The objective of this visit is for Dr. Ebiefung to work with Prof. Judice to develop a block principal pivoting algorithm for the vertical generalized complementarity problems (VGCP), when the associated matrix is a vertical block P-matrix. They are motivated by the efficiency of this method when applied to large scale problems in LCPs, especially that problems involving the VGCP are likely to be larger and more complex than what they have for the LCP. Dr. Ebiefung's research, though in an area with rich and practical applications, has been theoretical. Working with Prof. Judice will help him transition to large scale implementations of the algorithms he has developed in this area as well as provide me with the impetus to model and solve realistic practical problems in areas such as urban transportation, energy distribution, electrical networks, and water resource planning. While at UTC, Dr. Judice will deliver a seminar on the linear complementarity problem (LCP) and its

applications at the SimCenter. He also plans to give a series of lectures on solutions techniques of the LCP at the Department of Mathematics.

Requesting Faculty: Fernando Alda
Invited Speaker: Dr. Xingly Giam, University of Tennessee Knoxville
Lecture Title: Metaanalytic modeling of conservation ecology of freshwater fishes

Summary of Qualifications/Lecture:
Dr. Giam is an Assistant Professor in the Department of Ecology and Evolutionary Biology at the University of Tennessee-Knoxville. His research is focused on conservation ecology of freshwater systems combining fieldwork and experimental data with the development and application of cutting-edge theoretical, statistical, and metaanalytic modeling tools. Some examples of his work include projects in the southern Appalachians in the US and Indonesia that explore the impact of global change (climatic, anthropogenic) on biodiversity and its mitigation strategies, and the mechanisms underlying large-scale patterns of species diversity and distribution to inform regional and global conservation priorities. Overall, Dr. Giam conducts highly interdisciplinary and policy-relevant research across multiple spatial scales that is well-aligned with the interests of faculty and students of the Departments of Biology, Geology and Environmental Science, Mathematics and Computer Science, among others. Furthermore, Dr. Giam has a strong record of publications—over 45 articles published in peer-reviewed journals—and external grant funding of his research.

FY2020 Budget

NEW CORE AWARDS FY2020				
Investigators	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Sungwoo Yang	Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling	Energy & the Environment	$99,959	$98,551
Jared Pienkos	Alkynyl tetrafluoro-pyridyl ligands: computational studies, synthesis, and characterization	Health & Biological Systems	$73,832	$67,279**
Eleni Panagiotou, Jin Wang, Wang-Yong Yang, Chris Dowell, and Abi Arabshahi	A study on the local and global effects of polymer entanglement in material properties and biological functions	Health & Biological Systems	$99,941	$71,211**
Francesca Leasi, Jejal Bathi, Lani Gao, and Hong Qin	Simulating bio-environmental interactions using –omics approaches	Health & Biological Systems	$100,000	$90,000
Farah Kandah, Mina Sartipi	Decentralized and Scalable Trust Management Approach via Blockchain for Connected Vehicles in Smart Cities	Smart Cities & Urban Dynamics	$100,000	$62,019**
Hamdy Ibrahim, Mohammad Mahtabi	Corrosion modeling of magnesium-based fixation hardware for mandibular reconstruction surgeries	Health & Biological Systems	$99,906	$81,666**
Azad Hossain, Mark Schorr, and Jejal Bathi	Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies	Energy & the Environment	$96,488	$78,620**
Jennifer Hogg, Shellie Acocello, Gary Wilkerson, Yu Liang, and Dalei Wu	The Use of Augmented Reality–Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation	Health & Biological Systems	$90,538	$90,538
Bradley Harris, David Giles, and Chris Dowell	The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence	Health & Biological Systems	$92,742	$89,707**

NEW INITIATION/OPPORTUNITY AWARDS FY2020				
Investigators	**Project Title**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Fernando Alda	Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)	Health & Biological Systems	$24,949	$24,575
Ashley Manning-Berg	Modeling of microbial mat decay and implications for the early Earth fossil record	Health $ Biological Systems	$15,000	$2,300**
Stephanie DeVries	A Simplified Subsurface Characterization for Local-Scale Groundwater Flow Models in Unconfined Sand and Gravel Aquifers	Health & Biological Systems	$24,981	$20,707
Loren Hayes	Using computational approaches to enhance comparative studies of social evolution	Health & Biological Systems	$17,242	$14,805
Reetesh Ranjan	A multi-fidelity computational modeling strategy for large-eddy simulation of turbulent combustion	Aerospace & Defense	$25,000	$21,027**

** *Due to COVID-19, some or all of the remaining funds on projects marked with asterisks were approved as carryover into FY2021 to support student researchers.*

DISTINGUISHED LECTURE SERIES AWARDS FY2020				
UTC Faculty	**Invited Lecturer**	**CEACSE Priority Area**	**Amount Awarded**	**Amount Expended**
Fernando Alda	Dr. Xingli Giam	Health & Biological Systems	$400	$0
Aniekan Ebiefung	Dr. Joaquim João Júdice	High-Performance Computing & Algorithms	$3,000	$0

Note: Due to COVID-19 travel restrictions, neither of these awards were utilized in FY2020. They have been approved as carryover into FY2021.

Schedule 7

CENTERS OF EXCELLENCE ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution: UT Chattanooga

Center: Center of Excellence in Applied Computational Science & Engineering

	FY 2019-20 Actual			FY 2020-21 Proposed			FY 2021-22 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures									
Salaries									
Faculty	$118,911	$220,835	**$339,746**	$152,023	$282,328	**$434,351**	$133,394	$247,731	**$381,125**
Other Professional	$22,227	$41,279	**$63,505**	$28,416	$52,773	**$81,189**	$24,934	$46,306	**$71,240**
Clerical/ Supporting	$1,914	$3,554	**$5,468**	$2,447	$4,544	**$6,990**	$2,147	$3,987	**$6,134**
Assistantships	$74,164	$137,733	**$211,897**	$94,816	$176,086	**$270,902**	$83,197	$154,508	**$237,705**
Total Salaries	**$217,216**	**$403,401**	**$620,616**	**$277,702**	**$515,731**	**$793,433**	**$243,672**	**$452,533**	**$696,204**
Longevity	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Fringe Benefits	$30,544	$56,724	**$87,267**	$39,049	$72,519	**$111,568**	$34,264	$63,632	**$97,896**
Total Personnel	**$247,759**	**$460,124**	**$707,884**	**$316,750**	**$588,250**	**$905,000**	**$277,935**	**$516,165**	**$794,100**
Non-Personnel									
Travel	$1,911	$3,549	**$5,461**	$2,443	$4,538	**$6,981**	$2,144	$3,982	**$6,126**
Software	$16,195	$30,077	**$46,273**	$20,705	$38,453	**$59,158**	$18,168	$33,741	**$51,909**
Books & Journals			-	-	-	-	-	-	-
Other Supplies	$22,064	$40,976	**$63,040**	$28,208	$52,386	**$80,594**	$24,751	$45,966	**$70,718**
Equipment	$63,152	$117,283	**$180,436**	$80,738	$149,942	**$230,680**	$70,844	$131,568	**$202,412**
Maintenance			**$0**	$0	$0	**$0**	$0	$0	**$0**
Scholarships	$14,952	$27,769	**$42,721**	$19,116	$35,501	**$54,617**	$16,773	$31,151	**$47,924**
Consultants	-	-	-	-	-	-	-	-	-
Renovation	-	-	-	-	-	-	-	-	-
Other (Specify):			-			-			-
Print	$603	$1,120	**$1,722**	$771	$1,431	**$2,202**	$676	$1,256	**$1,932**
Other Personal Services	$2,258	$4,193	**$6,450**	$2,886	$5,360	**$8,246**	$2,532	$4,703	**$7,236**
Rentals	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Group Arranged Events	$0	$0	**$0**	$0	$0	**$0**	$0	$0	**$0**
Special Commercial Services	$6,629	$12,312	**$18,941**	$8,475	$15,740	**$24,215**	$7,437	$13,811	**$21,248**
Membership	$144	$267	**$411**	$184	$342	**$525**	$161	$300	**$461**
Student Fees	$11,232	$20,860	**$32,092**	$14,360	$26,668	**$41,028**	$12,600	$23,400	**$36,001**
Total Non-Personnel	**$139,141**	**$258,405**	**$397,546**	**$177,886**	**$330,360**	**$508,247**	**$156,088**	**$289,877**	**$445,965**
GRAND TOTAL	**$386,900**	**$718,530**	**$1,105,430**	**$494,637**	**$918,611**	**$1,413,247**	**$434,023**	**$806,043**	**$1,240,065**
Revenue									
New State Appropriation		$793,189	**$793,189**		$794,729	**$794,729**		$834,465	**$834,465**
Carryover State Appropriation		$76,847	**$76,847**		$151,507	**$151,507**		$0	-
New Matching Funds	$405,600		**$405,600**	$405,600		**$405,600**	$405,600		**$405,600**
Carryover from Previous Matching Funds	$42,712		**$42,712**	$61,412		**$61,412**	$0		**$0**
Total Revenue	**$448,312**	**$870,036**	**$1,318,348**	**$467,012**	**$946,236**	**$1,413,247**	**$405,600**	**$834,465**	**$1,240,065**

FY2020 PUBLICATIONS AND PRESENTATIONS (of CEACSE Seed-Funded Research)

Conference Presentations, Posters, and Proceedings

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Panagiotou, **E**., Topology Workshop, Institute of Advance Study, April 2020, UPenn

Panagiotou, **E**., SIAM Conference on Mathematical Aspects of Materials Science, May 2020, Bilbao, Spain

J. Wang, "Immersed boundary and immersed domain methods for fluid-structure interaction", Special Session on Applicable Analysis and Control Theory for Fluid and Fluid-Structure PDEs, SIAM
Panagiotou, **E**., Conference on Analysis of Partial Differential Equations, La Quinta, CA, December 2019.

Y. W. Wang, talk at SERMACS 2019, October 2019

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

Kandah, F. IEEE High Performance Extreme Computing Conference (HPEC)

Kandah, F. IEEE 9th Annual Computing and Communication Workshop and Conference (CCWC).

Kandah, F. UTC Research Dialogues.

Neglia, S.; Lee, J. P.; **Pienkos, J. A**. Synthesis, characterization, and reactivity of a heterobimetallic organometallic complex with a trans bidentate ligand for catalytic carbon-hydrogen bond activation. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Truong, T. T.; Mconkey, A. M.; Moser, Z. D.; McDarmont, S. L.; Lee, J. P.; Wang-Yong, Y.; **Pienkos, J. A.** Synthetic strategies for generating 4-ethynyl-2,3,5,6-tetrafluoropyridine. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Jaques, L. D.; McDarmont, S. L.; McMillen, C.; Neglia, S.; Lee, J. P.; **Pienkos, J. A.** Synthesis of tbpyPt(C22py)2 and its interactions with Cu(I) and Pd(II) metals. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

McDarmont, S. L.; Jaques, L. D., Synthesis of multi-metallic acetylide compounds of d10 transition metals. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Strike, W., Martin, D., Glass, K., **Harris, B.** Phospholipid remodeling via exogenous polyunsaturated fatty acid uptake modulates stress resistance in Vibrio cholerae. Poster presented at: AIChE National Conference; 2019 November 11; Orlando, FL.

Rojas, E., Giles, D., Wang, J., and **Harris, B**. Influence of population density and environmental conditions on *V. cholerae* growth and virulence. ASM Microbe 2020 June 18-22; Chicago, IL (abstract accepted for poster presentation, conference postponed).

Turgeson, A., **Harris, B.** Elucidation of the mechanism of long-chain fatty acid recognition in *V. cholerae*: an in silico study. American Institute of Chemical Engineers Annual Meeting 2020 November 15-20; San Francisco, CA (abstract accepted for conference paper).

Hogg, J., OPTIMAL-Based Virtual Reality Feedback to Reduce Dual-Task Balance Cost, 2020 Virtual Meeting of the American Society of Biomechanics (will be refereed in the Journal of Biomechanics)

Hogg, J., Research Dialogues (cancelled)

Harvey T, **Alda F** (2020) Revised phylogenetic hypothesis and comparative evolution of mitochondrial genomes of Neotropical weakly electric fishes (Gymnotiformes). *ReSEARCH Dialogues Conference Proceedings.*

Alda, F. 2020 Joint Meeting of Ichthyologists and Herpetologists (cancelled)

Harvey T, **Alda F.** 2020 Research Dialogues. Poster.

DeVries, S. Nitrate Model, Wisconsin Department of Natural Resources. 2020.

Suggs, E. 2019. Meta-analysis in biology research literature. Association for Computing Machinery.

Carpenter, **Hayes** and Tanis, presented (via Zoom) the automated search tool to unfunded collaborator Schradin's lab group, IPHC-Strasbourg, France.

R. Ranjan, "Application of reduced order modeling for simulation of turbulent combustion," Research Dialogues, 2020.

R. Ranjan, AIAA SciTech Forum and Exposition, 2020, Orlando, FL, USA.

Preyanka Dey, **Jejal Reddy Bathi**, "Watershed modeling techniques to understand impacts of pollutants on microbiology", EWRI Watershed Management Conference 2020, Henderson, Nevada, May 17- May 21, 2020. (Poster Presentation)

Preyanka Dey, **Jejal Reddy Bathi, Francesca Leasi** "Hydrologic models to evaluate pollutant's impacts on microbiology", Tennessee Water Resource Symposium, Montgomery Bell State Park, Burns, TN, April 22 – 24, 2020.

Preyanka Dey, **Jejal Reddy Bathi** "Hydrological Modeling for Watershed Management, Technology Symposium", Downtown Library, Chattanooga, Tennessee, April 17, 2020.

Preyanka Dey, **Jejal Reddy Bathi, Francesca Leasi** "Hydrological Modeling of South Chickamauga Creek watershed using BASINS/HSPF", TNSA Annual Conference Going the Distance in 2020. (Podium presentation)

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

Hossain, **A**., Blanton, R., and Mathias, C., Remote Sensing of Surface Water Quality in Southeast Tennessee. The manuscript is under preparation and to be submitted to Remote Sensing of the Environment.

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

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

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

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

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

Yang, S. “Thermal and Mechanical Properties of 3-Dimensional Carbon Network as Flexible Thermal Additives” (in progress, 50%).

Yang, S. “Optimization of The Adsorbent Geometries of Water Harvesting System by Finite Element Method” (in progress, 65%).

F. Kandah, B. Huber, A. Altarawneh, S. Medury and A. Skjellum, "BLAST: Blockchain-based Trust Management in Smart Cities and Connected Vehicles Setup," 2019 IEEE High Performance Extreme Computing Conference (HPEC), Waltham, MA, USA, 2019, pp. 1-7, doi: 10.1109/HPEC.2019.8916229.

F. Kandah, A. Altarawneh, B. Huber, A. Skjellum, and S. Medury, "A Human-Understandable, Behavior-based Trust Management Approach for IoT/CPS at Scale," Int. J. of International Society for Computers and Their Applications (ISCA), In Press (2020)

J. Coleman, **F. Kandah** and B. Huber, "Behavioral Model Anomaly Detection in Automatic Identification Systems (AIS)," 2020 10th Annual Computing and Communication Workshop and Conference (CCWC), Las Vegas, NV, USA, 2020, pp. 0481-0487, doi: 10.1109/CCWC47524.2020.9031248.

A. Altarawneh, T. Herschberg, S. Medury, **F. Kandah** and A. Skjellum, "Buterin's Scalability Trilemma viewed through a State-change-based Classification for Common Consensus Algorithms," 2020 10th Annual Computing and Communication Workshop and Conference (CCWC), Las Vegas, NV, USA, 2020, pp. 0727-0736, doi: 10.1109/CCWC47524.2020.9031204.

Jaques, L. D.; McDarmont, S. L.; Smart, M. M.; McMillen, C. D.; Neglia, S. E.; Lee, J. P.; **Pienkos, J. A.,** Structural characterization of the metalloligand tbpyPt(C22-py)2 and its interaction with Pd(OAc)2. *Inorganic Chemistry Communications* 2020, 112, 107722. (IF 1.943)

Pienkos, J.A., Exploiting a C-F activation Strategy to Generate Novel Tris(pyrazolyl)methane Ligands (submitted ZAAC, IF 1.24)

Hogg, J., Wellness Survey Responses and Smartphone App Response Efficiency Associate with Remote History of Sport-Related Concussion, Perceptual and Motor Skills (under review)

DeVries, S., Bradbury, K., and Cardiff, M. “A Groundwater Flow Model for Waupaca, WI.” Wisconsin Geological Survey and Natural History Survey Technical Report.

R. Ranjan, and S. Menon, “Application of Nonlinear Reduced Order Modeling Strategy for Large Eddy Simulation of Chemically Reacting Turbulent Flows”, AIAA-2020-2140, AIAA SciTech Forum and Exposition, 2020. (DOI: https://doi.org/10.2514/6.2020-2140)

R. Ranjan, Assessment of Two Level Simulation Model for Compressible Turbulent Mixing Layer, Accepted**,** 17th International Workshop on the Physics of Compressible Turbulent Mixing, Atlanta, USA, July 13-17, 2020.

R. Ranjan, Application of Hybrid Transported-Tabulated Chemistry for Efficient Large-Eddy Simulation of Turbulent Premixed Combustion, Under Review, AIAA SciTech Forum and Exposition, 2021.

Preyanka Dey, **Jejal Reddy Bathi**, **Francesca Leasi**, “Sensitivity of HSPF Model watershed hydrology for BASINS 4.5 Land Cover and Meteorological Databases” (manuscript under preparation)

EXTERNAL FUNDING

Azad Hossain, Lead PI

Co-PI(s): Jejal Reddy Bathi and Mark Schorr

Other Personnel: Richard Blanton, Caleb Mathias, Shuvashish Roy, and Syed Tareq
Project Title: "Integration of Satellite Observations with Numerical Watershed and Hydrodynamic Models for Surface Water Quality Studies"

Proposal Submissions

1. Integration of Remote Sensing Technology with Hydrodynamic Models for Surface Water Quality Monitoring in Southeast Tennessee, Agency: USGS through Tennessee Water Resources Research Center (TNWRRC). Duration: March 1, 2020 - February 28, 2021. Total amount: $24,976 (Federal) and $50,390 (Non-federal). Role: Principal Investigator. Not funded.
2. Urban Streams Restoration Project: Measuring the Efficacy of Habitat Mitigation/Restoration Efforts on Chattanooga Area Streams: Citico Creek, Friar Branch, and Mountain Creek. Agency: City of Chattanooga. Duration: 01/01 /2020 - 08/ 31/ 2022. Amount: $275,907. Role: Co-Principal Investigator (Principal Investigator: Mark Schorr). Pending.
3. Integration of remote sensing technology and numerical model for water quality study in Mississippi Sound. Agency: The Mississippi Based RESTORE Act Center of Excellence (MBRACE) at the University of Southern Mississippi. Duration: 01/01/2020 – 12/31/2021. Total amount: $87, 88. This proposal was submitted by The University of Mississippi in collaboration with The University of Tennessee at Chattanooga (UTC). Role: Co- Principal Investigator [UTC Principal Investigator]. Not Funded.

Contracts/Awards Received

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

Sponsored Program Capacity Building Activities

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

Eleni Panagiotou, Lead PI

Co-PI(s): Jin Wang, Abi Arabshahi, W. Y. Yang, Chris Dowell
Other Personnel: Evan Gildernew

Project Title: "Polymer Entanglement"

Proposal Submissions

1. NSF Proposal on Entanglement in Polymers submitted prior to reporting period but immediately related to the proposed work.
2. NSF CAREER: Topology of the cytoskeleton (not funded)
3. NSF MODULUS (not funded)

4. ORAU Powe award (pending)

Contracts/Awards Received

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

Sponsored Program Capacity Building Activities

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

Hamdy Ibrahim, Lead PI

Co-PI(s): Mohammad Mahtabi

Project Title: "Corrosion Modeling of Magnesium-Based Fixation Hardware For Mandibular Reconstruction Surgeries"

Proposal Submissions

1. Ibrahim, H., "Treating Bone Trauma Using ResorbFix", I-Corps Teams, submitted to the National Science Foundation (NSF), 2020. Requested amount: $50,000.
2. Ibrahim, H., Mahtabi, M., Danquah, M., Elliot, T., Palchoudhury, S., Elliot, L. & Panagiotou, E. "Acquisition of a customized metal additive manufacturing system for multidisciplinary research activities", Major Research Instrumentation Program: (MRI), submitted to the National Science Foundation (NSF), 2020. Requested amount: $261,500.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Sungwoo Yang, Lead PI

Co-PI(s): N/A
Project Title: Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling"

Proposal Submissions

1. Submitted a proposal, $1.4M, (concept paper) for the DARPA call on Atmospheric Water Extraction (AWE, HR001120S0014), but not selected.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

1. CAREER preparation workshop & CAREER panels meeting to receive their comments
2. Nghia Chiem, Licensing Associate, University of Tennessee Research Foundation
3. SimCenter Energy Thrust at UTC
4. Jeffrey B Cornett, Manager, Industrial Partnerships & Economic Development at ORNL
5. Kashif Nawaz, Senior Research Scientist at ORNL

Farah Kandah, Lead PI

Co-PI(s): Mina Sartipi

Project Title: "Decentralized and Scalable Trust Management Approach Via Blockchain for Connected Vehicles in Smart Cities."

Proposal Submissions

1. NSF EAGER
2. NSF SaTC
3. NSF CCRI

Contracts/Awards Received

N/A

Sponsored Program Capacity-Building Activities

1. A number of meetings were held with the grant administrator at SimCenter in support of our ongoing proposal. These meetings included reviewing our proposal, providing guidance and directions which were very beneficial in creating a well written proposal.
2. The graphic designed personnel was very helpful at different occasions during the development of our external proposals.

Jared A. Pienkos, Lead PI

Co-PI(s): Dr. Wang-Yong Yang and Dr. John P. Lee

Other Personnel: Dr. Colin McMillen, Dr. James Burgess, Dr. Paul S. Wagenknecht, Dr. Berhane Temelso, Tracie Durham.

Project Title: "Alkynyl Tetrafluoro-Pyridyl Ligands: Computational Studies, Synthesis, and Characterization"

Proposal Submissions

1. ACS PRF- Exploiting Metallohinged *Trans*-bidentate Ligands for Suzuki Coupling
2. NSF REU- Exploiting Pyridyl-based Ligands and Secondary Site Interactions in Transition Metal Alkynyl Compounds
3. NSF Career- Exploiting Halogen-Bonding to Tune to Optical Properties of Transition Metals for Their Use in Organic Light Emitting Diodes.

Contracts/Awards Received

N/A

Sponsored Program Capacity-Building Activities

N/A

Bradley Harris, Lead PI

Co-PI(s): David Giles

Other Personnel: Andrew Turgeson, Konner Glass, Devin Martin, Diane Madeksho, Dalton Strike, Christopher Dowell

Project Title: "The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence"

Proposal Submissions

1. NSF CAREER, CAREER: Developing a mechanistic model for unsaturated fatty acid recognition in Gram-negative bacteria ($519,000, 2/1/21-1/31/25)

Contracts/Awards Received

1. NIH R15 Award #1R15GM131315-01A1, Experimentally Guided Modeling and Simulation for Cholera Dynamics ($340,000, 9/1/19-8/31/22)

Sponsored Program Capacity Building Activities

1. Prepared NSF CAREER proposal draft for external reviewers secured by UTC's Office of Research and Sponsored Programs.
2. Virtual meeting with Dr. David Rockcliffe, PO for NSF BIO MCB Systems and Synthetic Biology cluster.

Francesca Leasi, Lead PI

Co-PI(s): Jejal Bathi, Lani Gao, Hong Qin

Project Title: Simulating bio-environmental interactions using –omics approaches

Proposal Submissions

1. 2020. Ruth S. Holmberg Grants for Faculty Excellence. University of Tennessee at Chattanooga. Funded
2. 2020. Faculty Achievement Award. College of Arts & Sciences. University of Tennessee at Chattanooga. Funded
3. 2020. NSF CAREER Program – Division of Environmental Biology. Under Review
4. 2019. NSF– Division of Environmental Biology. Declined
5. 2019. NSF – MRI. Declined

Contracts/Awards Received

1. 2020. $4,800. PI. "Biodiversity of Microscopic Invertebrates in Hamilton County Using Cutting-edge Molecular Approaches". Ruth S. Holmberg Grants for Faculty Excellence. University of Tennessee at Chattanooga.
2. 2020. $1,000. PI. "Smithsonian Marine Station (SMS) Meiofauna Diversity and Taxonomy Workshop". Faculty Achievement Award. College of Arts & Sciences. University of Tennessee at Chattanooga.

Sponsored Program Capacity Building Activities

N/A

Jennifer Hogg, Lead PI

Co-PI(s): Shellie Acocello, Yu Liang, Dalei Wu, Gary Wilkerson

Project Title: "The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"

Proposal Submissions

1. An R15 AREA NIH proposal entitled “A New Paradigm for Sport Injury Prevention and Reduction of Risk for Disability” that was submitted in February 2020 included the CEACSE project PI (Jennifer Hogg) as a co-researcher and one of the participating researchers as PI (Gary Wilkerson). A review summary statement was recently received that included very good reviewer scores, which suggests that the potential for funding of a revised proposal is promising. A revision is currently being prepared for submission in October, which includes a Computer Engineering faculty member as a co-investigator (Mina Sartipi, PhD).

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Fernando Alda, Lead PI

Project Title: “Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)”

Proposal Submissions

1. UT Collaboration Grant

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

1. Attended the CAREER grant preparation workshop organized at UTC by T.I.G
2. Met with Ashley Ledford, Grants Administrator from the College of Arts and Science to discuss funding opportunities.

Ashley Manning-Berg, Lead PI

Project Title: “Modeling of microbial mat decay and implications for the early Earth fossil record”

Proposal Submissions

N/A

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Stephanie DeVries, Lead PI

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

Proposal Submissions

N/A

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

Loren Hayes, Lead PI

Other Personnel: Craig Tanis

Project Title: "Using Computational Approaches to Enhance Comparative Studies of Social Evolution"

Proposal Submissions

1. FY2020-2021 Center of Excellence in Applied Computational Science & Engineering (CEACSE): Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models (co-PI, Dr. Craig Tanis, UTC College of Engineering). Funding: $98,662.
2. National Science Foundation**:** Comparative and computational analyses of climatic and life history drivers of variable social organization in mammals. (PI: Loren Hayes, co-PIs Craig Tanis & Jin Wang, $610,809). Proposal no. 2037549, submitted in June 2020.

Contracts/Awards Received

1. FY2020-2021 Center of Excellence in Applied Computational Science & Engineering (CEACSE): Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models (co-PI, Dr. Craig Tanis, UTC College of Engineering). Funding: $98,662.
2. National Science Foundation (#1854177): Collaborative Research: IRES Track I: Stronger together: Exploring how communal care reduces individual costs during challenging years (2019-2022; PI: Loren Hayes; co-PIs, Shewanee Howard-Baptiste, & Jennifer Ellis). Funding: $263,356 (In collaboration with Dr. Carolyn Bauer, total award = $399,968). Note: This award was made in August 2019. Although not directly related to the project, it is possible that I could use this funding to support computational work with collaborators in Chile.

Sponsored Program Capacity Building Activities

1. Hayes met with NSF IOS and OISE program officers at NSF offices (Virginia) in February 2020.

Reteesh Ranjan, Lead PI

Project Title: "A Multi-Fidelity Computational Modeling Strategy for Large-Eddy Simulation of Turbulent Combustion"

Proposal Submissions

Following white papers and proposals have been submitted related to this award

1. A Data-Driven Multi-Parameter Reduced Order Modeling Framework for Investigation of Hypersonic Systems (White Paper, AFOSR # FOA-AFRL-AFOSR-2020-0002, Topic #26)
2. An Integrated Approach for Characterization and Predictive Modeling of Non-Equilibrium High Speed Turbulent Reacting Flows (White Paper, ONR Announcement # N00014-20-S-F003, Topic #9)
3. Low Emission combustor system for high overall pressure ratio compact core engines (Stage A Proposal, NASA ULI, Ultra-Efficient Subsonic Transports, Strategic Thrust 3)
4. Modeling Impact of Wind Turbulence on Autonomous Vehicles (Proposal, One UT Collaboration & Innovation Grant)
5. COVID-19-Relevant Computational Modeling of Human Respiratory Airways (Proposal, DOD IIRA W81XWH-20-PRMRP-IIRA-COV)

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

1. Attended the NSF CAREER proposal webinar.

OVERVIEW OF FY2021 PROJECTS

The following awardees and projects, selected for funding in February 2020, are currently supporting CEACSE's strategic goals and future plans for FY2021. All funded projects were subject to double-blind external peer review, followed by internal panel review in which the external review scores were the driving factor in determining final awards. This process ensures high caliber of funded projects and encourages higher-quality proposals in later competitions. It also has the added benefit of increasing the visibility of UTC and SimCenter outside of Tennessee and planting seeds of possible large-scale collaborations.

Core Competition

Title: A Low-Cost, Passive Solar Process Heat System
Investigators: Sungwoo Yang
Thrust: Energy
Amount: $82,771

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Faculty Initiation/Opportunity Award

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

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

CONCLUSION

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

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

CEACSE-supported initiatives have already formed the basis of several collaborations and partnerships with other institutions of higher education and with business and industry partners. A number of meaningful Memoranda of Understanding and Non-Disclosure Agreements have been executed between UTC and a variety of partners and potential sponsors to explore how CEACSE can support engineering enhancements, address regional and state priority areas, and bolster robust economic growth. Our strategic partnerships with organizations in Chattanooga and the larger region, such as the Enterprise Center, the CO.LAB, and the Chamber of Commerce have already resulted in increased NSF funds at UTC for CSE-related projects leveraging the Smart-connected GigCity status of Chattanooga.

In conclusion, advancing computational science and engineering to strengthen the education, workforce development, and R&D missions at UTC continues to be a high-value investment for the State of Tennessee and the U.S. The CEACSE multidisciplinary team of faculty and graduate students in collaboration with their strategic partners in Chattanooga, the region, and elsewhere has been focused on the three primary objectives for the Center listed in the introductory segment of this report, namely to

- Expand CSE capabilities at UTC,
- Support startup of new research and educational work that broadens and expands the CEACSE base of research expertise, and
- Realize appropriate return on investment by attracting new extramural funding.

We are convinced that the work accomplished in FY2020 and the strategic vision we have laid out for the future have positioned UTC and CEACSE to continue to positively impact, enhance, and accelerate the growth and advancement of Tennessee's scientific and engineering capabilities and resources.

LEADERSHIP CONTACT INFORMATION AND BIOS

Dr. Joanne G. Romagni

Vice Chancellor for Research & Dean of the Graduate School
Joanne-Romagni@utc.edu

Dr. Joanne Romagni is the Vice Chancellor for Research and Dean of the Graduate School at UTC. Before joining UTC, she was the Associate Vice President for Research at DePaul University in Chicago, where she also served as a research fellow in the biology department. Previously, she held a variety of faculty and leadership positions in research and administration at Bucknell, St. Edwards, and St. Thomas Universities. She received her PhD in plant biology from Arizona State University and conducted research as a postdoctoral plant physiologist and biochemist at the USDA-ARS in Oxford, Mississippi.

In her current role, Dr. Romagni leads efforts at UTC to establish external and interdisciplinary research partnerships to advance the university's strategic plan. Her work develops the structures and support mechanisms to enhance and expand research across graduate and undergraduate disciplines at UTC. Under her leadership, proposal dollars requested have increased by more than $12 million. In FY20, external awards were up by nearly 15% compared to FY19, and Dr. Romagni initiated and administered more than $1,800,000 in internal grant awards.

Dr. Romagni approaches her work with a dedication to synergistic collaboration and strives to provide opportunities to underrepresented individuals. She personally mentored over 75 students in her previous lab, 80% of which were either women and/or Hispanic students. She has developed strong relationships and has extensive experience working with major grant-making agencies, having served on numerous federal review panels. She was awarded funds from the National Science Foundation for her work as a PI developing an international research program for undergraduates. She has been invited by the Association of American Colleges and Universities and the International Conference of Education, Research and Innovation to speak about her expertise and success integrating undergraduate research into curricula.

Dr. Anthony Skjellum

Director of the UTC SimCenter
Chair of Excellence in Applied Computational Science & Engineering
Tony-Skjellum@utc.edu

Dr. Anthony (Tony) Skjellum received his BS, MS, and PhD Degrees from Caltech. His PhD work emphasized portable, parallel algorithms and software for simulation, with a specific emphasis on message-passing systems. After graduating in 1990, he worked at LLNL for 2.5 years as a computer scientist, emphasizing performance-portable message passing and portable parallel math libraries. From 1993-2003, he was on faculty at Mississippi State University, where he and his students co-developed MPICH with Argonne National Laboratory, the first implementation of the now-pervasive Message Passing Interface (MPI-1) standard. Skjellum was a leading participant in MPI-1 and MPI-2 standards as well, with specific contributions to the concepts of "groups, contexts, and communicators," which stemmed from his PhD research. His work on MPI has made broad impact on all HPC worldwide through the MPICH implementation and further R&D on MPI over the past 25 years.

From 2003-2013, he was professor and chair at the University of Alabama at Birmingham (UAB), Department of Computer and Information Sciences, where he continued work on HPC and cyber. During his tenure at UAB, he co-founded a university-wide center, Center for Information

Assurance and Joint Forensic Sciences (CIA-JFR), together with Justice Science and Business leaders. This highly funded center was able to attract world-class cybersecurity and forensics researchers. It also spun-off a startup company, Malcovery, which was later acquired by PhishMe and still has a growing presence in Birmingham as of Fall 2018. In July 2014, he was appointed the Lead Cyber Scientist for Auburn University and Cyber Center director. He led the R&D in HPC and cyber at Auburn University in the College of Engineering for just over three years prior to joining the University of Tennessee at Chattanooga in August 2017 as a Professor of Computer Science, Chair of Excellence, and the new SimCenter Director.

Skjellum's current research group is a split between cyber/Internet of Things and HPC and Exascale Storage. FA-MPI is Skjellum's second implementation of a resilient MPI; he and students and his company, MPI Software Technology, previously designed and published MPI/FT, a fault-aware MPI based on MPI/Pro, a commercial MPI licensed from the mid-1990's through mid-2000’s. He has current funding from DOE/NNSA and NSF. He is a senior member of ACM and IEEE and Associate Member of the American Academy of Forensic Science (AAFS), Digital & Multimedia Sciences Division. Skjellum remains active in the MPI Forum (in multiple working groups) and is the former chair of the Object Management Group (OMG) High Performance Embedded Working Group as well, in which he remains actively involved as a standards designer and standardizer for high-performance embedded signal and image processing libraries and related application programmer interfaces.

Appendix A
Faculty Biosketches

Shellie Acocello, PhD, ATC
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518 Oak St.
Chattanooga, TN 37403
Shellie-Acocello@utc.edu
423-425-5798

(a) Professional Preparation

Louisiana College	Pineville, LA	Athletic Training	BS, 2008
Baylor University	Waco, TX	Athletic Training	MSEd, 2010
University of Virginia	Charlottesville, VA	Sports Medicine	PhD, 2014

(b) Appointments

- 2014 - Assistant Professor, Health & Human Performance, University of Tennessee Chattanooga
- 2012 – 2014 Research & Teaching Graduate Assistant, Athletic Training/Kinesiology, UVA
- 2010 – 2012 Head Athletic Trainer, St. Anne's Belfield School, Charlottesville, VA
- 2008 – 2010 Teaching Graduate Assistant, Athletic Training, Baylor University
- 2008 – 2010 Graduate Assistant Athletic Trainer, Football, Baylor University

(c) Publications

- **Acocello S***, Broshek DK, Saliba S. (2014) Inter-rater and intra-rater reliability of cerebral blood flow measures obtained using the brain acoustic monitor. *Journal of Neuroscience Methods*: 221:85-91.

- Partner S, Sutherlin MA, **Acocello S**, Saliba SA, Hart JM. (2014) Changes in muscle thickness after exercise and biofeedback in people with low back pain. *J Sport Rehab:* 23(4): 307-318.

- Meuthing A, **Acocello S***, Pritchard K, Saliba S, Hart JM. (2015) Shoulder muscle activation in individuals with previous shoulder injuries. *J Sport Rehab*. 24(3):278-285.

- Wilkerson GB, Grooms DR, **Acocello S**. (2017) Neuromechanical considerations for post-concussion musculoskeletal injury risk management. CSMR. 16(6):419-427.

- Hansberger B, **Acocello S**, Slater L, Hart J, Ambegaonkar J. Peak lower extremity landing kinematics in dancers and non-dancers. *J Ath Train*. In press.

(d) Synergistic Activities

- Proposal review for National Athletic Trainers' Association Annual Symposium, 2017 – Present
- Assists in coordination of graduate student research involving injury risk screening of Olympic, college, and high school athletes
- Member, Tennessee Athletic Trainers' Society Professional Education Committee, 2016 - Present
- Presented research annually at National Athletic Trainers' Association Annual Symposium via Free Communications Program, 2011 – Present.
- Experienced in neurocognitive assessment utilizing various tools of both computerized and paper-and-pencil formats

Biographical Sketch

Fernando Alda-Pons, Ph.D.
Assistant Professor

Dpt. Biology, Geology and Enviornmental Science
The University of Tennessee at Chattanooga
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fernando-alda@utc.edu; fernandoalda.weebly.com

(a) Professional Preparation

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

(b) Appointments

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

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

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

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

Picq S, **Alda F**, Bermingham E, Krahe R. 2016. Drift-driven evolution of electric signals in a Neotropical knifefish. Evolution 70: 2134-2144.

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

Alda F, Picq S, De León Reina LF, González R, Waltz H, Bermingham E, Krahe R. 2013. First record of *Gymnotus henni* in Panama, phylogenetic position and electric signal characterization. Check List 9: 655-659.

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

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

Alda F, Adams AJ, Chakrabarty P, McMillan WO. 2018. Mitogenomic divergence between three pairs of putative geminate fishes from Panama. Mitochondrial DNA Part B 3: 1-5.

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

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

Alda F, Adams AJ, McMillan WO, Chakrabarty P.2017. Complete mitochondrial genomes of three Neotropical sleeper gobies: *Eleotris amblyopsis*, *Eleotris picta* and *Hemieleotris latifasciata*. Mitochondrial DNA Part B 2: 747-750.

(d) Synergistic Activities

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

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

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

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

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University of Tennessee at Chattanooga | Chattanooga, TN 37403
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A. Professional Preparation:

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

B. Appointments:

2005 – Present	Research Professor University of Tennessee at Chattanooga
2002 – 2005	Associate Research Professor University of Tennessee at Chattanooga
1997 – 2002	Senior Research Associate Applied Research Laboratory, The Pennsylvania State University
1995 – 1997	Research Engineer II, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University
1991 - 1995	Research Engineer I, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University
1989 – 1991	Post-doctoral Fellow, Computational Fluid Dynamics Laboratory, NSF/ERC for Computational Field Simulation, Mississippi State University

C. Selected Recent Publications

i) Five publications most closely related to proposed project:

- Palchoudhury, S., Arabshahi, A., Gharge, U., Albattah, A., George, O., and Foster, Y., "Integrated Experimental and Computational Fluid Dynamics Approach for Nanoparticle Flow Analysis," submitted to the Journal of Materials Research, JMR-2018-0493, June 1, 2018.
- Palchoudhury, S., Jungjohann, K., Weerasena, L., Arabshahi, A., Gharge, U., Albattah, A., Miller, J., Patel, K., and Holler, R., "*Enhanced legume root growth with pre-soaking in α-Fe_2O_3 nanoparticle fertilizer*," Royal Society of Chemistry Advances Journal, 2018. 8: pp. 24075-24083.
- Azarnoosh, J., Sreenivas, K., Arabshahi, A., "CFD Investigation of Human Tidal Breathing through Human Airway Geometry," Procedia Computer Science, Vol.80, pp. 965-976, 2016.
- Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Simulation of Airflow and Particle Deposition in the Lungs," Poster Presentation, 2014 UT Institute of Biomedical Engineering Symposium, Knoxville, TN , April 2014.
- Whitfield, D. L., Taylor, L. K., Beddhu, M., and Arabshahi, A., "Discretized Newton- Relaxation Solution of the Three-Dimensional Unsteady Incompressible Navier-Stokes Equations," *Frontiers of Computational Fluid Dynamics,* Chapter 28, pp. 575-594, D. A. Caughey and M. M. Hafez, Editors, ISBN 0-471-95334-2, John Wiley & Sons, Ltd., New York, 1994.

ii) Five other significant publications:

- Hasbestan, J.J., Newman III, J.C., and Arabshahi, A., "Least Squares Spectral Element Method For Laminar Compressible Flows," AIAA Science and Technology Forum and Exposition (SciTech 2016) San Diego, California, January 4-8, 2016.

- Gruetzemacher, R., Arabshahi, A."Effects of Inhalation Transience on Particle Transport Through a CT-Based Human Airway Geometry," IMECE2015-52606, to be presented at International Mechanical Engineering Congress and Exhibition, Houston, TX, November 13-19, 2015.
- Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Effects of Inhalation Transcience on Flow Structures During Numerical Simulation of Airflow through a CT-Based Airway Geometry," Summer Biomechanics, Bioengineering and Biotransport Conference (SB3C), Snowbird Resort, Utah, June 17-20, 2015.
- Gruetzemacher, R., Arabshahi, A., and Sreenivas, K., "Numerical Simulation of Airflow in a CT-based Human Airway Model With Physiologically Appropriate Boundary Conditions," Poster Presentation within the Respiratory Bioengineering Track, Biomedical Engineering Society Annual Meeting, San Antonio, Texas, October 2014..
- Arabshahi, A., Janus, J. M., "A Multiblock Compressible Navier-Stokes Flow Solver Applied to Complex Launch Vehicles," *AIAA Journal of Spacecraft and Rockets*, Vol. 41, No. 3, pp. 469-472, May-June 2004.

D. Synergistic Activities:

- SimCenter leadership role in unsteady viscous flow engineering applications, scientific computing, and structured grid technologies, including software development, integration, and management, and also facilitating teamwork to solve complex real-world engineering problems (University of Tennessee at Chattanooga)
- SimCenter leadership role in high-performance cluster computing, including cluster design, benchmarking, acquisition, and resource allocation (University of Tennessee at Chattanooga)
- Thesis Advisor for one Undergraduate Honor Student and one MS Student (University of Tennessee at Chattanooga)
- Committee member for 7 MS and 3 PhD students (Mississippi State University) and for 6 MS and 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.”

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A. Professional Preparation:

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

Appointments:

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

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

1. Bathi, J.R., and H.S. Das**.,** 2016. **"**Vulnerability of Coastal Communities from Storm Surge and Flood Disasters," International Journal of Environmental Research and Public Health, Vol. 13, pp 239.
2. Bathi, J.R., 2016, Village Creek Watershed SWMM Model Report, Village Creek Watershed Improvement Plan. A technical report submitted to the City of Birmingham, AL.
3. Pitt, R., K. Goodson, O. Ogburn, V. Eppakayala, Bathi, J.R., Wilson, B., Subramaniam, S., and Clark, S., 2013. "Identification and Treatment of Emerging Contaminants in Wet Weather Flows," EPA Contract: EP-C-07-014. Office of Research, EPA. (Research Report)
4. Bathi, J. R., R.E. Pitt, and S.E. Clark., 2012. "Polycyclic aromatic hydrocarbons in urban stream sediments," Advances in Civil Engineering.
5. Pitt, R. Pitt., S. E. Clark, Y. Cai, M. Renee and Bathi, J.R., 2017. "Southeastern United States Observations of Stormwater Pollutant Strengths by Particle Size," Journal of Water Management Modeling, 2017, DOI: 10.14796/JWMM.C418.

5 Other Significant Publications:

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

Synergistic Activities (up to 5):

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

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a. Professional Preparation

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

b. Appointments

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

c. Publications

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

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

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

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

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

d. Synergistic Activities

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

e. Collaborators & Other Affiliations

(i)Collaborators

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

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

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

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

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

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

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

(ii) Graduate and Postdoctoral Advisors

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

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

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

f. Research Impacts

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

Cuilan (Lani) Gao, PhD

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PROFESSIONAL PREPARATION

• Wuhan Textile University	Textile Engineering	B.S.,	1996-2000
• University of Mississippi	Statistics	Ph.D.,	2005-2010
• St Jude Children's Research Hospital	Biostatistics	Postdoc.,	2010-2012

APPOINTMENTS

- 2017-Present, Associate Professor, Dept. of Mathematics**,** University of Tennessee at Chattanooga
- 2012-2017, Assistant Professor, Dept. of Mathematics**,** University of Tennessee at Chattanooga
- 2014-Present, Biostatistics Faculty, The University of Tennessee College of Medicine at Chattanooga

PUBLICATIONS AND PROJECTS

(i) Five most closely related to the proposal project

1) Manish Tripathi and C. Gao, "Z Probe, an Efficient Tool for Characterizing Long Non-Coding RNA in FFPE Tissues", *Journal of Non-Coding RNA*, Special Issue 4-20, 2018.
2) L. Zhu, S. Pounds, C. Gao and R. Gilbertson et al., "Multi-organ mapping of cancer risk", *Cell*, 166(5):1132-1146, 2016.
3) C. Gao and B. Shamsaei, "Comparison of machine learning and statistical algorithms for Classification of human cancer type", *IEEE Engineering in Medicine and Biology Society*, 978-1-5090-2455-1, pp.296-299, 2016.
4) D. Kawauchi and C. Gao and etc. "A mouse model for the most aggressive molecule subtype of human Medulloblastoma", *Cancer Cell*, vol. 21 (2), pp. 168-180, 2012.
5) S. Pounds, C. Gao, "Empirical Bayesian selection of hypothesis testing procedures for analysis of mRNA-seq data", *Statistical Applications in Genetics and Molecular Biology*, Vo.5, pp.1544-115(2013).

(ii) Five other significant publications

1) Y. Liang, D. Wu, W. Wu and C. Gao "Big Data-enabled Multiscale Serviceability Analysis about Aging Bridges", Journal of Digital Communications and Networks, vol. 2 (3), pp. 97-107, 2016.
2) C. Gao, C. Cheng, "A phenotype-drive dimension reduction (PhDDR) approach to integrated genomic association analysis", *IEEE Engineering in medicine and Biology Society*, pp.6837-40(2011).
3) S. Pounds, C. Gao, R. Johnson, K. Wright, H. Poppleton, D. Finkelstein, S. Leary and R. Gilbertson, "A procedure to statistically evaluate agreement of differential expression for cross-species genomics", *Bioinformatics*, 27 (15), pp.2098-2103 (2011).
4) C. Murphy, B. Foster and C. Gao, "Temporal Dynamics in Rhizosphere Bacterial Communities of Three Perennial Grassland Species", *Multidisciplinary Digital Publishing Institute Agronomy* 2016, 6, 17.
5) C. Gao, X. Dang, Y. Chen and D. Wilkins. "Graph ranking for exploratory gene data analysis", *BMC Bioinformatics* 10 (Suppl. 11): S19(2009).

SYNERGISTIC ACTIVITIES

1) Gao is currently investigating NSF founded program I-MATH (2015-2018) as Co-PI. The major goal of I-MATH program is to train undergraduate and graduate students with strong interdisciplinary knowledge and skills, and provide them with new education and research experiences that will promote their career development in the STEM fields The program encompasses a breadth of applied and computational mathematics, statistics, biology, computer science, and engineering. In summer 2016, Gao was co- leading one-week summer camp which was successfully conducted. Around 25 best students from high schools in TN were enrolled in the program. Gao led the statistical session during the summer camp and trained the students by lectures and hands-on projects on how to use statistical software to conduct data analysis and big data analysis in math lab.
2) Gao is a recipient of 2017 CORNET (Collaborative Research Network in Cancer) award across UT campuses. The project studies a divergent trend in mortality rates between African American and Caucasians with colorectal cancer over the last 40 years. The Gao-Tripathi team is looking at cellular and molecular mechanisms that dictate how the disease behaves and progresses in underserved populations.
3) Gao is also a recipient of UTC Ruth S. Holmberg Grant for Faculty Excellence Award (2015), the grant is about classification of subtypes of cancers using neural networks and cross species genomic data. One paper based on this method was recently published by *Jacob Journal of Biostatistics*. Latest Gao was selected as the recipient of Research and Creativity Grant from College of Arts and Science at UTC. She was also the winner of 2016 University of Tennessee Outstanding Teacher.
4) Gao has been working as a statistical consultant for the University of Tennessee College of Medicine where she provides statistical methods, data analysis at the forefront and consults on planning experiment design of clinical trial studies. Furthermore, Gao trains the medical residents by giving statistical lectures at research seminars each year.

COLLABORATORS & OTHER AFFILIATIONS

(i) Collaborators

Dr. Richard Gilbertson, MD, Professor and Director of Head of Dept. of Oncology, Director, Cambridge Cancer Center CRUK Cambridge Institute.
Dr. Jin Wang, professor, Department of Mathematics at University of Tennessee at Chattanooga;
Dr. Loren Hayes, Associate Professor, Department of Biology at University of Tennessee at Chattanooga
Dr. Stan Pounds, Ph.D., associate Professor in Department of Biostatistics, at St. Jude Children's Research Hospital.
Dr. Paul Dassow, MD, Associate Professor in Family Medicine at Erlanger Hospital;
Dr. Greg W. Heath, professor of the University of Tennessee at Chattanooga and Director of UT College of Medicine at Chattanooga
Dr. Yu Cao, Ph.D., associate Professor in Department of Computer Science at the University of Massachusetts Lowell.

(ii) Advising and Mentoring

Dr. Gao has advised numerous undergraduate students and graduate students including one undergraduate honor thesis and one graduate students who won the Provost Student Award, as well as high school junior/seniors via three consecutive three years' I-MATH project funded by NSF.

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a. Professional Preparation

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

b. Appointments

- Associate Professor, Department of Biology, Geology & Environmental Science, Aug. 2018 – present.
- Assistant Professor, Department of Biology, Geology & Environmental Science, Aug. 2012 – 2018
- Lecturer, Human Infectious Diseases, The University of Texas at Austin, Spring 2012

c. Publications (10 out 20)

i) Five publications most closely related to proposed project:

- Baker, L. Y., C. R. Hobby, A. W. Siv, W. C. Bible, M. S. Glennon, D. M. Anderson, S. J. Symes and D. K. Giles. 2018. *Pseudomonas aeruginosa* responds to exogenous polyunsaturated fatty acids (PUFAs) by modifying phospholipid composition, membrane permeability, and phenotypes associated with virulence. *BMC Microbiology* 18:117. doi: 10.1186/s12866-018-1259-8
- Hobby, C. R., J. L. Herndon, C. A. Morrow, S. J. K. Symes and D. K. Giles. 2018. Exogenous fatty acids alter phospholipid composition, membrane permeability, capacity for biofilm formation and antimicrobial peptide susceptibility in *Klebsiella pneumoniae*. *MicrobiologyOpen*: e00635.
- Eder, A. E., S. A. Munir, C. R. Hobby, D. M. Anderson, J. L. Herndon, A. W. Siv, S. J. K. Symes and D. K. Giles. 2017. Exogenous polyunsaturated fatty acids (PUFAs) alter phospholipid composition, membrane permeability, biofilm formation and motility in *Acinetobacter baumannii*. *Microbiology* 163: 1626-1636.
- Moravec, A. R., A. W. Siv, C. R. Hobby, E. N. Lindsay, L. V. Norbash, D. J. Shults, S. J. K. Symes and D. K. Giles. 2017. Exogenous polyunsaturated fatty acids impact membrane remodeling and affect virulence phenotypes among pathogenic *Vibrio* species. *Appl. Environ. Microbiol.* 83: e1415-17.
- Giles, D.K., J. V. Hankins, Z. Guan, and M. S. Trent. 2011. Remodeling of the *Vibrio cholerae* membrane by incorporation of exogenous fatty acids from host and aquatic environments. *Mol. Micro*. 79: 716-728.

ii) Five other significant publications:

- Needham, B. D., S. M. Carroll, D. K. Giles, G. Georgiou, M. Whiteley and M. S. Trent. 2013. Modulating the innate immune response by combinatorial engineering of endotoxin. *Proc. Natl. Sci. USA*. 110: 1464-1449.
- Pride, A. C., C. M. Herrera, Z. Guan, D. K. Giles and M. S. Trent. 2013. The outer surface lipoprotein VolA mediates utilization of exogenous lipids by *Vibrio cholerae*. *mBio* 4: e00305-13.
- Maue, A., K. Mohawk, D. K. Giles**,** F. Poly, C. P. Ewing, Y. Jiao, G. Lee, Z. Ma, M. A. Monteiro, C. L. Hill, J. S. Ferderber, C. K. Porter, M. S. Trent, and P. Guerry. 2013. The polysaccharide capsule of *Campylobacter jejuni* 81-176 modulates the host immune response. *Infect. Immun.* 81: 665-672.
- Hankins, J. V., J. A. Madsen, D. K. Giles, J. S. Brodbelt and M. S. Trent. 2012. Amino acid addition to *Vibrio cholerae* LPS establishes a link between surface remodeling in Gram negative and Gram positive bacteria. *Proc*. *Natl. Acad. Sci. USA.* 109: 8722-8727.
- Cullen, T. W., D. K. Giles, L. N. Wolf, C. Ecobichon, I. G. Boneca, and M. S. Trent. 2011.

Helicobacter pylori versus the host: Remodeling of the bacterial outer membrane is required for survival in the gastric mucosa. *PLoS Pathog*. 7: e1002454.

d. Synergistic Activities

- **Co-PI, NSF award** #1520672, "I-Math: Interdisciplinary Math Program". Dr. Giles' responsibilities include lectures and laboratories for college students, as well as participation in summer I-MATH camp, an interdisciplinary collection of lectures and exercises for high school students.
- **Co-PI** on an internally funded grant to mathematically and experimentally model *Vibrio cholerae* dynamics to assess contributing factors of disease dissemination and epidemiology
- **Co-PI** on an internally funded grant involving bioreactor-scale simulation of the biphasic lifestyle of *Vibrio cholerae* to study the impact of exogenous fatty acids
- **Co-PI** on two internally funded grants involving the characterization of methicillin-resistant *Staphylococcus aureus* from Erlanger Children's Hospital in Chattanooga, TN.
- **Undergraduate Research Advisees:** 28 total since 2012; Three have completed M.S. and one is pursuing M.S.; Nine undergraduates have received internal grants for their research; Three undergraduates have won presentation awards at regional meetings; Fourteen undergraduates earned co-authorship on published manuscripts.

Biographical Sketch

Bradley Harris
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(a) Professional Preparation

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

(b) Appointments

2015 – Present University of Tennessee at Chattanooga, Assistant Professor
2010 – 2014 University of Tennessee at Knoxville, Graduate Research Assistant

(c) Publications

(i) Most Closely Related Products

1. Harris, B., Cheng, X., and Frymier, P.D. Structure and function of photosystem I- [FeFe] hydrogenase protein fusions: An all-atom molecular dynamics study. *Journal of Physical Chemistry B* **2016**, 120(4), p. 599-609.
2. Harris, B., Cheng, X., and Frymier, P.D. All-atom molecular dynamics simulation of a photosystem I/detergent complex. *Journal of Physical Chemistry B* **2014**, 118(40), p. 11633-11645.
3. Le, R., Harris, B., Iwuchukwu, I.J., Bruce, B., Cheng, X., Qian, S., Heller, W.T., O'Neill, H., and Frymier, P.D. Analysis of the solution structure of *Thermosynechococcus elongatus* photosystem I in *n*-dodecyl-*β*-D-maltoside detergent using small-angle neutron scattering and molecular dynamics simulation. *Archives of Biochemistry and Biophysics* **2014**, 550-551, p. 50-57.
4. Harris, B., Le, R., and Frymier, P.D. Characterizing the structure-function relationship that governs electron transport in redox proteins. *Abstracts of Papers of the American Chemical Society* **2014**, 247.
5. Harris, B. and Frymier, P.D. Harnessing solar energy through enzyme-mediated protein fusions. *Abstracts of Papers of the American Chemical Society* **2013**, 245.

(d) Synergistic Activities

- **NSF S-STEM Award** # 1741695, "UTC ASSETS: Academic Intervention, Social Supports, and Scholarships for Engineering Transfer Students." Dr. Harris is co-PI on an S-STEM award providing scholarships to transfer students. His responsibilities include oversight of the faculty and peer mentor programs, and he is also the industry liaison and professional development coordinator.
- **Interdisciplinary approach to research through bioengineering**. Dr. Harris' research involves the application of chemical engineering principles to biological problems. One current research project on the environmental adaptations of bacterial pathogens is in collaboration with the Dept. of Biology and the SimCenter at UTC, and has been funded by multiple internal awards.
- **Demonstration of hands-on projects to local high school teachers**. Dr. Harris seeks to engage local high school and community college students in chemical engineering through hands-on demonstrations and remote labs. He has organized

hands-on workshops for Future Ready Institute initiatives as well as UTC College of Engineering and Computer Science open house events. He is also actively working to bring online lab stations involving unit operations such as absorption, distillation, heat transfer, fluid flow, and reaction kinetics through the use of internet of things.

- **Development of curricular materials for laboratory courses**. Dr. Harris developed a bioreactor station for junior- and senior-level chemical engineering laboratory courses in collaboration with Dr. Giles from UTC Dept. of Biology. This work was presented at the American Society for Engineering Education Southeastern Section conference in 2018.
- **Collaboration with local industry on senior design projects**. Dr. Harris organizes industry-sponsored projects for the chemical engineering senior design course at UTC in collaboration with local industry partners, including BASF, Chattem Chemicals, Colonial Chemical, TVA, and W.R. Grace and Co.

BIOSKETCH FOR LOREN D. HAYES

A. Professional preparation

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

B. Appointments

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

C. Products

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

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

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

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

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

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

(ii) Five other products (=student)*

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

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

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

(9) Hofmann, H.A., Beery, A.K., Blumstein, D.T., Couzin, I.D., Earley, R.L, **Hayes, L.D.,** Hurd, P.L., Lacey, E.A., Phelps, S., Solomon, N.G., Taborsky, M., Young, L.J., & Rubenstein, D.R. 2015. An evolutionary framework for studying mechanisms of social behavior. *Trends in Ecology & Evolution,* 29, 581-589.

(10) **Hayes, L. D.,** Correa, L. A., Abades, S., Gao, C. L., & Ebensperger, L. A. 2018. Male group members are costly to plurally breeding *Octodon degus* females. *Behaviour*, *1*(aop), 1-36.

D. Synergistic activities

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

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

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

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

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

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(a) Professional Preparation

Troy University	Troy, AL	Athletic Training	BS, 2006
University of Alabama	Tuscaloosa, AL	Health Studies	MA, 2008
UNC-Greensboro	Greensboro, NC	Applied Neuromechanics	PhD, 2018

(b) Appointments

2018 - Assistant Professor, Health & Human Performance, University of Tennessee Chattanooga
2017 – 2018 Lecturer, Health & Human Performance, University of Tennessee Chattanooga
2013 – 2017 Research & Teaching Graduate Assistant, Kinesiology, UNC-Greensboro
2008 – 2013 Head Athletic Trainer, Gulf Coast State College, Panama City, FL
2009 – 2012 Adjunct Instructor, Gulf Coast State College, Panama City, FL

(c) Publications

Hogg JA, Schmitz RJ, Nguyen A-D, Shultz SJ. (2018) Passive Hip Range of Motion Values Across Sex and Sport. *Journal of Athletic Training*. 53(6), 560-567

Hogg JA, Ackerman TA, Nguyen A-D, Ross SE, Schmitz RJ, Vanrenterghem J, Shultz SJ. The Effects of Gluteal Function on the Relationship between Femoral Alignment and Functional Valgus Collapse. (In review, *Journal of Athletic Training*).

Hogg JA, Ackerman TA, Nguyen A-D, Ross SE, Schmitz RJ, Vanrenterghem J, Shultz SJ. (2018) The Influence of Femoral Structure, Hip Capsular Constraints, and Gluteal Muscle Strength and Activation on Temporal Patterns of Functional Valgus Collapse. *Proquest Dissertations and Theses.*

Hogg JA, Shelton Z, Schmitz RJ, Shultz SJ. (2017) Neuromechanical Differences During a Single-Leg Forward Landing in Females with High and Low Hip Internal Rotation Range of Motion. *Journal of Athletic Training*. 52(6), S90-91.

(d) Synergistic Activities

Statistical Parametric Mapping for Biomechanics workshop attendee. March 31 – April 1, 2016. John Moores University, Liverpool, United Kingdom

ACL Research Retreat VII organizer, March 19 – 21, 2015. Greensboro, North Carolina

Developer and writer of textbook ancillary materials. Shultz SJ, Houglum, PA, & Perrin, DH. Examination of Musculoskeletal Injuries Presentation Package (CD ROM). 2015. Human Kinetics: Champaign, IL.

Peer Reviewer for *Journal of Clinical Medicine Research*, 2018.

Peer Reviewer for *Journal of Dance Medicine & Science*, 2018.

(e) Collaborators and other Affiliations
12 total collaborators
Ackerman TA, College of Education, University of Iowa
Acocello S, Department of Health & Human Performance, University of Tennessee at Chattanooga
Diekfuss J, Cincinnati Children's Hospital Medical Center, Cincinnati, OH
Liang Y, Department of Computer Science & Engineering, University of Tennessee at Chattanooga
Nguyen A-D, Department of Exercise Science, High Point University
Ross SE, Department of Kinesiology, University of North Carolina Greensboro
Schmitz RJ, Department of Kinesiology, University of North Carolina at Greensboro
Shultz SJ, Department of Kinesiology, University of North Carolina Greensboro
Vanrenterghem, J, Catholic University of Leuven, Flanders, Belgium
Waxman JP, Department of Exercise Science, High Point University
Wilkerson GW, Department of Health & Human Performance, University of Tennessee at Chattanooga
Wu D, Department of Computer Science & Engineering, University of Tennessee at Chattanooga

Graduate Advisor
Sandra J. Shultz, Professor, Department of Kinesiology, Co-Director, Applied Neuromechanics Research Laboratory, University of North Carolina, Greensboro

Hamdy Ibrahim
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Tel: 423-425-4718
Email: hamdy-ibrahim@utc.edu

(a) Professional Preparation

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

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

(c) Products

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

- **Ibrahim, H.** and Elahinia, M. *Process to Produce High-Strength and Corrosion Resistant Alloy for Patient-Specific Bioresorbable Bone Fixation Implants and Hardware*. *WO2017112779A1*, December 21, 2015.
- **Ibrahim, H**., Jahadakbar, A., Dehghan, A., Moghaddam, N. S., Amerinatanzi, A., & Elahinia, M. (2018). *In Vitro Corrosion Assessment of Additively Manufactured Porous NiTi Structures for Bone Fixation Applications*. Metals, 8(3), 164.
- **Ibrahim, H.**, Klarner, A. D., Poorganji, B., Dean, D., Luo, A. A., & Elahinia, M. (2017). *Microstructural, mechanical and corrosion characteristics of heat-treated Mg-1.2 Zn-0.5 Ca (wt%) alloy for use as resorbable bone fixation material*. Journal of the mechanical behavior of biomedical materials, 69, 203-212.
- **Ibrahim, H.**, Esfahani, S. N., Poorganji, B., Dean, D., & Elahinia, M. (2017). *Resorbable bone fixation alloys, forming, and post-fabrication treatments*. Materials Science and Engineering: C, 70, 870-888.
- Amerinatanzi, A., Moghaddam, N. S., **Ibrahim, H.**, & Elahinia, M. (2016, September). *Evaluating a NiTi implant under realistic loads: A simulation study*. In ASME 2016 Conference on Smart Materials, Adaptive Structures and Intelligent Systems (pp. V002T03A030-V002T03A030). American Society of Mechanical Engineers.

(ii) Five other significant products:

- Cooper J.C., Elahinia, M., Gupta, R. & **Ibrahim, H.** Minimally Invasive Thrombectomy Device. CIP, US20150265299A1, April 2, 2015.
- **Ibrahim, H**., Mehanny, S., Darwish, L., & Farag, M. (2018). *A comparative study on the mechanical and biodegradation characteristics of starch-based composites reinforced with different lignocellulosic fibers*. Journal of Polymers and the Environment, 26(6), 2434-2447.
- **Ibrahim, H.**, Farag, M., Megahed, H., & Mehanny, S. (2014). *Characteristics of starch-based biodegradable composites reinforced with date palm and flax fibers*. Carbohydrate polymers, 101, 11-19.

- Ma, C., Andani, M. T., Qin, H., Moghaddam, N. S., **Ibrahim, H.**, Jahadakbar, A., Amerinatanzi, A., Ren, Z., Zhang, H., Doll, G.L., & Dong, Y. (2017). *Improving surface finish and wear resistance of additive manufactured nickel-titanium by ultrasonic nano-crystal surface modification*. Journal of Materials Processing Technology, 249, 433-440.
- Moghaddam, N. S., Saghaian, S. E., Amerinatanzi, A., **Ibrahim, H.**, Li, P., Toker, G. P., Karaca, H. E., & Elahinia, M. (2018). Anisotropic tensile and actuation properties of NiTi fabricated with selective laser melting. Materials Science and Engineering: A, 724, 220-230.

(d) Synergistic Activities

- **Professional Services:** Dr. Ibrahim served as a 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.

- **Technology Commercialization:** Dr. Ibrahim was integral to 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.

- **Editorial:** Dr. Ibrahim currently serves as a guest editor for Special Issue titled "Engineering Bone-Implant Materials" in the MDPI – Bioengineering Journal. Dr. Ibrahim also serves as a 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.*

- **Mentees: Dr. Ibrahim** mentored 2 undergraduate students in senior year research projects and 2 graduate students through their master's thesis projects.

Farah Kandah

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University of Tennessee at Chattanooga
735 Vine Street
Chattanooga, TN 37405

a. Professional Preparation

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

b. Appointments

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

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

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

c.ii. Other Significant Publications

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

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

d. Synergistic Activities

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

Biographical Sketch

Francesca Leasi
University of Tennessee at Chattanooga
Department of Biology, Geology, and Environmental Science
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a. Professional Preparation

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

b. Appointments

- Assistant Professor at Department of Biology, Geology & Environmental Science, University of Tennessee at Chattanooga, August 2018 – present.
- Research Associate at Department of Molecular, Cellular, and Biomedical Sciences, University of New Hampshire, Durham, NH, August 2017 – July 2018.
- Research Fellow at Department of Invertebrate Zoology, Smithsonian Institution National Museum of Natural History, Washington D.C., February 2013 – June 2017.
- Research Fellow at Academy of Natural Sciences of Drexel University, Philadelphia, PA, February 2012 – February 2013.
- Research Associate at Division of Population Biology, Imperial College London, UK, February 2011 – January 2012.
- Postdoctoral Fellow at Department of Biology, University of Milan, Italy, June 2007 – May 2010.

c. Publications *Asterisks indicate undergraduate co-authors*

i) Five publications most closely related to proposed project:

- Leasi F, Sevigny J, Laflamme EM, Artois T, Curini-Galletti M, de Jesus Navarrete A, Di Domenico M, Goetz F, Hall JA, Hochberg R, Jörger KM, Jondelius U, Todaro MA, Wirshing HH, Norenburg JL, Thomas WK (In Press) Biodiversity estimates and ecological interpretations of meiofaunal communities are biased by the taxonomic approach. *Nature Communications Biology*. DOI: 10.1038/s42003-018-0119-2.
- Martínez-Arce A*, De Jesús-Navarrete A, González-Medina E, Leasi F (Accepted) COI gene and algorithmic analyses for species delimitation in marine nematodes. *Thalassas: An International Journal of Marine Sciences.*
- Leasi F, Andrade S, Norenburg JL (2016) At least some meiofaunal species are not everywhere. Indication of geographic, ecological and geological barriers affecting the dispersion of species of Ototyphlonemertes (Nemertea, Hoplonemertea). *Molecular Ecology 25:1381-1397. DOI:10.1111/mec.13568.*
- Leasi F, Gaynus C*, Mahardini A*, Moore NT*, Norenburg JL, Barber HP (2016) Spatial and ecological distribution of neglected microinvertebrate communities across endangered ecosystems: Meiofauna in Bali (Indonesia). *Marine Ecology* 37: 970-987. DOI:10.1111/maec.12305
- Curini-Galletti M, Artois T, Delogu V, De Smet WH , Fontaneto D, Jondelius U, Leasi F, Martínez A, Meyer-Wachsmuth I, Nilsson KS, Tongiorgi P, Worsaae K, Todaro MA (2012) Patterns of diversity in soft-bodied meiofauna: dispersal ability and body size matter. *PLoS ONE* 7: e33801. DOI:10.1371/journal.pone.0033801.

ii) Five other significant publications:

- Leasi F, Norenburg JL (2014) The necessity of DNA taxonomy to reveal cryptic diversity and spatial distribution of meiofauna, with a focus on Nemertea. *PLoS ONE* 9(8):

e104385. DOI:10.1371/journal.pone.0104385.
- Leasi F & De Smet W (Accepted) Rotifer distribution at different salinities in the United States with the description of two new species. *Hydrobiologia*
- Mills S, Alcántara-Rodríguez JA, Ciros-Pérez J, Gómez A, Hagiwara A, Galindo KH, Jersabek CD, Malekzadeh-Viayeh R, Leasi F, Lee JS, Mark Welch DB, Papakostas S, Riss S, Segers H, Serra M, Shiel R, Smolak R, Snell TW, Stelzer CP, Tang CQ, Wallace RL, Fontaneto D, Walsh EJ (2017) Fifteen species in one: deciphering the *Brachionus plicatilis* species complex (Rotifera, Monogononta) through DNA taxonomy. *Hydrobiologia* 796: 39-58. DOI:10.1007/s10750-016-2725-7.
- Leasi F, Tang CQ, De Smet WH, Fontaneto D (2013) Cryptic diversity with wide salinity tolerance in the putative euryhaline *Testudinella clypeata* (Rotifera, Monogononta). *Zoological Journal of the Linnean Society* 168:17-28. DOI:10.1111/zoj.12020.
- Tang CQ, Leasi F, Obertegger U, Kieneke A, Barraclough TG, Fontaneto D (2012) The widely used small subunit 18S rDNA molecule greatly underestimates true diversity in biodiversity surveys of the meiofauna. *Proceedings of the National Academy of Sciences of the United States of America* 109: 16208-16212. DOI:10.1073/pnas.1209160109

d. Synergistic Activities

- Session Chair for the Symposium "*Measuring Biodiversity and Extinction – Present and Past".* SICB conference, San Francisco, Jan 3-7, 2018.
- Co-Organizer of the II Benthic Invertebrate Taxonomy, Metagenomics, and Bioinformatics Workshop (BITMaB). Harte Institute Texas A&M Corpus Christi. January 2018.
- Master Thesis Dissertation Committee for the Environmental Engineering Department. University of New Hampshire. Fall 2018.
- Co-Organizer of the II Benthic Invertebrate Taxonomy, Metagenomics, and Bioinformatics Workshop (BITMaB). Harte Institute Texas A&M Corpus Christi. January 2017.
- Organizer and PI of the Meiofauna Workshop. Achotines Bay (Panama). February – March 2016.

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(a) Professional Preparation

University of Tennessee at Chattanooga	Chattanooga, TN	Chemistry	B.A. 2003
North Carolina State University	Raleigh, NC	Chemistry	Ph.D. 2008
University of Tennessee at Chattanooga	Chattanooga, TN	Postdoc	2010

(b) Appointments

Associate Professor, Chemistry, University of Tennessee at Chattanooga, TN	2017-Present
Assistant Professor, Chemistry, University of Tennessee at Chattanooga, TN	2012-2017
Post-Doctoral Fellow, Chemistry, University of Tennessee at Chattanooga, TN	2010-2012
Research & Development Chemist, Eastman Chemical Company, Longview, TX	2010-2012

(c) Products

1. J. P. Lee; T. P. Latendresse; K. R. Henson; P. A. Dean; L. F. Mehne "Synthetic, Electrochemical, Spectroscopic, and Structural Studies of Mixed Sandwich Co(III) Complexes Containing Involving Cp or Cp* with Tridentate N-Donor and S-Donor Macrocycles." *Inorganica Chimica Acta*, **2018**, Accepted

2. T. P. Latendresse; S. A. Adams; G. J. Grant; J. P. Lee; A. G. Oliver "Synthetic and Structural Studies of Heteroleptic Platinum(II) and Palladium(II) Complexes Containing Thiacrown and Monodentate Phosphane Ligands." *Polyhedron*, **2016**, 14, 80. Invited Contribution to a Special Issue on Undergraduate Research in Inorganic Chemistry.

3. J. P. Lee; M. J. Hankins; A. D. Riner; T. V. Albu "Synthetic, Structural, and Spectroscopic Studies of Mixed Sandwich Ru(II) Complexes Involving η^6-p-cymene and either Monodentate Fluorine-Containing Phosphines or Phosphites." *Journal of Coordination Chemistry*, **2016**, 69, 20.

4. J. P. Lee; C. L. Keller; A. A. Werlein; D. E. Janzen; D. E. VanDerveer; G. J. Grant "C-H Bond Activation by a Palladium(II) Thioether Complex: Formation of the Bis(nitromethanate) Complex $[Pd(9S3)(CH_2NO_2)_2]$." *Organometallics*, **2012**, 31, 6505. Accepted as Cover Art for Issue 18

5. J. P. Lee; G. J. Grant; B. N. Noll "Bis(1,4,7-trithiacyclononane)nickel(II) bis(tetrafluoridoborate) nitromethane solvate." *Acta Crystallographica*, **2011**, E67, m1417.

6. B. A. McKeown; J. P. Lee; J. Mej; T. R. Cundari; T. B. Gunnoe "Transition Metal Mediated C-H Activation and Functionalization: The Role of Poly(pyrazolyl)borate and Poly(pyrazolyl)alkane Ligands." *European Journal of Inorganic Chemistry*, **2016**, 2296. Invited Micro-Review to a Special Issue on the 50th Anniversary of the Discovery of Scorpionate Ligands.

7. S. Delp; L. Goj; C. Munro-Leighton; J. P. Lee; T. B. Gunnoe; T. R. Cundari; J. L. Petersen "Well-Defined Cu(I) Amido Complex and Aryl Iodides Reacting to Form Aryl Amines." *Organometallics*, **2011**, 30, 55.

8. N. A. Foley; J. P. Lee; Z. Ke; T. B. Gunnoe; T. R. Cundari "Ru(II) Catalaysts Supported by Hydridotris(pyrazolyl)borate for the Hydroarylation of Olefins: Reaction Scope, Mechanistic Studies, and Guides for the Development of Improved Catalysts." *Accounts of Chemical Research*, **2009**, 42, 585.

9. J. P. Lee; Z. Ke; M. A. Ramirez; T. B. Gunnoe; T. R. Cundari; P. D. Boyle; J. L. Petersen "Six- Five-, and Four-Coordinate Ruthenium(II) Hydride Complexes Supported by N-Heterocyclic Carbene Ligands: Synthesis, Characterization, Fundamental Reactivity, and Catalytic Hydrogenation of Olefins, Aldehydes, and Ketones." *Organometallics*, **2009**, 28, 1758.

(d) Synergistic Activities

1. Undergraduate research: The UTC Department of Chemistry and Physics is well recognized for a quality research program involving undergraduate majors. The main research activity, the summer Undergraduate Research Program, is supported through the Grote Chemistry fund. Dr. Lee has supervising 12 students over 6 summers since he joined UTC as an Assistant Professor in 2012. This has resulted in 3 peer-reviewed publications (with undergraduate student co-authors), 5 student-given presentations and 3 presentations given by Dr. Lee at conferences and Universities in the past 2 years.

2. URP program: Dr. Lee has participating the organization of the Department's summer URP for the past 3 years. This involves all organization leading up (i.e., during the fall and spring semesters) to the program and during the summer. Prior to the summer, Dr. Lee organizes the application process, and the at the end of the summer organizes a departmental poster session (open to the campus) in preparation for the students to present their work at a conferences. During the summer, Dr. Lee organizes the meetings, student presentations, inviting a summer speaker, tours of local chemical industry and workshops on campus such as Endnote tutorials done through the library

3. Book publication: J. P. Lee "Engaging Students in the Inorganic Chemistry Classroom with Well-Defined Learning Activities and Literature Discussions. In Addressing the Millenial Student: New Pedagogy and Approaches to Improve Student Learning Outcomes in Undergraduate Chemistry." C. R. Dockery and G. E. Potts, editors, ACS Symposium Series, 2014, American Chemical Society: Washington, DC, 1180, 25.

4. Website contributions: Since 2012 seven learning objects have been contributed to the Virtual Inorganic Pedagogical Electronic Resource (VIPEr), which is a production of the Interactive Online Network of Inorganic Chemists (IONiC) at www.ionicviper.org.

5. SERMACS symposium: At the 2017 Southeastern Regional Meeting of the American Chemical Society (SERMACS), Dr. Lee organized an invited symposium entitled "Undergraduate Research and Teaching at the Frontiers of Inorganic Chemistry." This involved planning, inviting and fundraising (to cover speaker expenses). Six speakers participated in the teaching/pedagogy half of the full-day symposium, and 7 speakers participated in the research half. The speakers ranged from research-intensive Ph.D. granting institutions to large public PUI's to small private PUI schools all with a focus on undergraduate education and research in the field of inorganic chemistry. At the 2017 Southeastern Regional Meeting of the American Chemical Society (SERMACS), Dr. Lee organized general inorganic oral abstracts that were submitted in response to the call for papers.

Yu LIANG, PhD (Computer Science), PhD (Applied Mathematics)
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Dr. Yu Liang is currently working at the Department of Computer Science and Engineering of University of Tennessee at Chattanooga as an Associate Professor. His funded research projects cover the following areas: modeling and simulation, high-performance scientific and engineering computing, numerical linear algebra, the processing and analysis of large-scale sensory data, and computational mechanics. His research work has appeared in various prestigious journals, book and book chapters, and refereed conference, workshop, and symposium proceedings. Besides two NSF review panels, Dr. Liang is serving in the Journal of Mathematical Research and Applications (JMRA), Current Advances in Mathematics (CAM), and the International Journal of Security Technology for Smart Device (IJSTSD) as an editorial board member.

A. PROFESSIONAL PREPARATION

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

B. APPOINTMENT

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

C. PUBLICATIONS:

(i) Five most closely related to proposal project

- **Y. Liang**, D. Wu, Z. Guo, C. Davis, D. Ledesma, and R. Slaughter, "Virtual Tai-Chi, System, a Smart Connected Modality for Rehabilitation", Smart Health, July 2018, DOI: 10.1016/j.smhl.2018.07.021.
- **Y. Liang,** D. Wu, G. Liu, Y. Li, L. Gao, and W. Wu, *Big Data-enabled Multiscale Serviceability Analysis about Aging Bridges*, Elsevier Digital Communications and Networks Journal. August 2016, 97-107. DOI: 10.1016/j.dcan.2016.05.002.
- **Y. Liang** and C. Wu, *A HADOOP-Enabled Sensor-Oriented Information System for Knowledge Discovery about Target-of-interest*, Internet of things - special issue of FUEE Scientific Journal (Impact Factor: 0.460), Vol. 29, No. 3, March 2016, 437-450.
- **Y. Liang,** M. Szularz and L. T. Yang, *Finite-element-wise Domain Decomposition Iterative Solvers Based on Polynomial Preconditioning*, DOI: 10.1016/j.mcm.2012.11.017, Mathematical and Computer Modeling (Impact Factor: 1.346). Vol. 58, Issues 1–2, July 2013, Pages 421-437.
- **Y. Liang**, and Z. Shi, *A Hessian-Free Newton-Raphson Method for the Configuration of Physics Systems Featured by Numerically Asymmetric Force Field*, Mathematical and Computer Simulation, (Impact Factor: 1.109), DOI: 10.1016/j.matcom.2016.11.011 (on press).

(ii) Five other significant publications

- **Y. Liang**, J. Weston and M. Szularz, *Generalized Least-squares Polynomial Preconditioners for Symmetric Indefinite Linear Equations*. Parallel computing (Impact Factor: 1.311), 28(2): 323-341 (2002).
- R. Mohan, Y. Purohit, **Y. Liang**, *Deformation Behavior of Nanoscale Material Systems with Applications to Tensile, Flexural and Crack Propagation*, Journal of Computational and Theoretical Nanoscience (Impact Factor: 0.911), Volume 9, Number 5, May 2012, pp. 649-661(13). **DOI:** 10.1166/jctn.2012.2075.
- J. Zhang, **Y. Liang** and Y. Zhang, *Atomic-level Protein Structure Refinement Using Fragment guided Molecular Dynamics Conformation Sampling*. Structure (Impact factor: 6.347), Vol.19, 1784–1795, December 2011.
- J. Zhang, **Y. Liang**, J.Z. Yan and J. Z. Lou, *Study of the molecular weight dependence of glass transition temperature for amorphous poly (L-lactide) by molecular dynamics simulation*, Polymers (Impact Factor: 3.438), Volume 48, Issue 16, 27 July 2007, 4900-4905.
- **Y. Liang**, S. Li, H. Zhang and C.D. Han, *Timing Sequence Testing for parallel Programs*, Journal of Computer Science and Technology (Impact factor: 0.678), 84-95. Jan. 2000.

D. SYNERGISTIC ACTIVITIES

- Panel for NSF Smart Connected Community (SC&C) and NSF Graduate Research Fellowships Program (GRFP) since 2015.
- Program Committee Member, the 2019 IEEE Big Data Service (March 26-29, 2018. Seattle, USA, http://www.big-dataservice.net/)
- Program Committee Member, the 2018 IEEE Big Data Service (March 26-29, 2018. Bamberg, Germany, http://www.big-dataservice.net/)
- Program Committee Member, the 2017 IEEE International Conference on Smart City Innovations (August 4-8, 2017, San Francisco, USA, http://ieee-smartworld.org/2017/sci/).
- Review panelist for the 2015-2017 NSF Graduate Research Fellowship Program (GRFP).
- Editorial Board Member of the International Journal of Security Technology for Smart Device (IJSTSD, URL:http://www.sersc.org/journals/IJSTSD/), Journal of Mathematical Research and Applications (JMRA), and Current Advances in Mathematics (CAM).
- Member of Editorial Board and Program Committee Member, First International Workshop on Security Technology for Smart Device (STSD 2015), URL: http://interworkshop.org/STSD2015.
- Member of Editorial Board, Journal of Mathematical Research and Applications, URL: http://www.academicpub.org/jmra/ .
- Technique Program Committee member of the Embedded Computing and Systems Track, the 6th International Conference on Frontier of Computer Science and Technology (FCST 2011: http://trust.csu.edu.cn/conference/fcst2011/)
- Reviewer of “Sensor”, “Supercomputing”, “Journal of Applied Mathematics and Computer Science”, “Journal of Parallel and Distributed Computing”, and “Parallel Computing”.

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a) Professional Preparation

Institution	Major/Area	Degree, Year
University of Tehran (Tehran, Iran)	Engineering/ Civil	B.Sc., 2005
Iran Univ. of Sci. & Tech. (Tehran, Iran)	Engineering/ Civil	M.Sc. 2008
Mississippi State Univ. (MS, USA)	Engineering/ Mechanical	Ph.D., 2017
University of Toledo (OH, USA)	Additive Manufacturing, Shape Memory Alloys, Fatigue and Fracture	PostDoc, 2017

b) Appointments

08/2018-present Assistant Professor, ME Department, UT Chattanooga, TN, USA
09/2017-07/2018 Postdoc, MIME Department, The University of Toledo, OH, USA

c) Products

i. Five most closely related to the proposal

- **Mahtabi, M.J.**, Stone T.W. and Shamsaei N., Load sequence effects and variable amplitude fatigue of superelastic NiTi. *International Journal of Mechanical Sciences*, 148 (2018): 307-315.
- Bagheri, A., **Mahtabi, M.J.** and Shamsaei, N., Fatigue behavior and cyclic deformation of additive manufactured NiTi. *Journal of Materials Processing Technology*, 252 (2018): 440-453.
- **Mahtabi M.J.** and Shamsaei N., Fatigue modeling for superelastic NiTi considering cyclic deformation and load ratio effects, *Shape Memory and Superelasticity* 3 (2017): 250-263.
- **Mahtabi M.J.**, Shamsaei N., and Mitchell, M.R., Fatigue of Nitinol: The state-of-the-art and ongoing challenges, *Journal of the Mechanical Behavior of Biomedical Materials* 50 (2015): 228–254.
- Saghaian S. E., Nematollahi M., Shayesteh Moghaddam N., Saedi S., Lu C. L., **Mahtabi M. J.**, Elahinia M., Karaca H. E, Effects of laser power and hatch spacing on the microstructure and shape memory response of SLM fabricated NiTi. *Submitted for publication.*

ii. Five other significant products

- Shao S., **Mahtabi M.J.**, Shamsaei N., and Thompson S.M., Solubility of argon in laser additive manufactured α-titanium under hot isostatic pressing condition. *Computational Materials Science* 131 (2017): 209-219.
- **Mahtabi M.J.** and Shamsaei N., A modified energy-based approach for fatigue life prediction of superelastic NiTi in presence of tensile mean strain and stress, *International Journal of Mechanical Sciences* 117 (2016): 321-333.
- **Mahtabi M.J.**, Shamsaei N., and Rutherford B., Mean strain effects on the fatigue behavior of superelastic Nitinol alloys: an experimental investigation, *Journal of Procedia Engineering* 133 (2015): 646–654.

- **Mahtabi M.J.** and Shamsaei N., Multiaxial fatigue modeling for Nitinol shape memory alloys under in-phase loading, *Journal of the Mechanical Behavior of Biomedical Materials*, 55 (2016): 236–249.
- Yadollahi, A., **M. J. Mahtabi**, A. Khalili, H. R. Doude, and J. C. Newman Jr., Fatigue life prediction of additively manufactured material: Effects of surface roughness, defect size, and shape, Fatigue & Fracture of Engineering Materials & Structures 41, No. 7 (2018): 1602-1614.

d) Synergistic Activities

- **Professional Services:** Dr. Mahtabi served as a member of the organization committee for "Advanced Manufacturing, Processing, Characterization, and Modeling of Functional Materials" symposium of Materials Science & Technology 2018. (MS&T 18), Columbus, OH. He is also a member of the ASTM Collaboration Team WK56674 - Revision of E466 Standard Practice for Conducting Force-Controlled Constant Amplitude Axial Fatigue Tests of Metallic Materials.

- **Editorial:** Dr. Mahtabi serves as a guest editor for Bioengineering Journal's special issue entitled "Engineering Bone- Implant Materials" in the MDPI –. Dr. Mahtabi also serves as a reviewer for several high impact journals, including *Fatigue & Fracture of Engineering Materials & Structures* and *Shape Memory and Superelasticity*.

- **Mentorship:** Dr. Mahtabi has advised a Masters student (Nazanin Farjam, 2018 in University of Toledo, co-advised with Prof. M. Elahinia). He has also mentored three PhD students at Dynamic and Smart Systems Lab at The University of Toledo as well as three graduate and three undergraduate students at Mississippi State University to perform research on the mechanical behavior of materials.

NSF Biographic Sketch
Ashley Manning-Berg

Professional Preparation

University of West Georgia	Geology	B.S., 2009
University of Tennessee, Knoxville	Geology	M.S., 2014
University of Tennessee, Knoxville	Geology	Ph.D., 2018

Appointments

Starting August 1, 2019 Assistant Professor, Biology, Geology, and Environmental Sciences University of Tennessee at Chattanooga
2018-2019 Visiting Professor, Earth, Environmental, and Planetary Sciences,
Case Western Reserve University
2012-2018 Graduate Teaching Assistant, Earth and Planetary Sciences,
University of Tennessee at Knoxville
2017 Graduate Research Intern, Planetary Geochemistry, The NASA Jet Propulsion Laboratory
2013 Geology Intern, ExxonMobil
2009-2011 Research Geologist, Geotechnical Engineering and Structures Laboratory,
U.S. Army Corps of Engineers – Engineer Research and Development Center

Publications

Publications most closely related to proposal project

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

Manning-Berg, A.R., Williford, K.H., and Kah, L.C. 2018. Evaluation of preliminary techniques used to assess taphonomic variation in silicified microbial mats preserved in the Angmaat Formation, northern Baffin Island, Nunavut Taphonomic assessment of silicified Mesoproterozoic microbial mats, in Summary of Activities 2018, Canada-Nunavut Geoscience Office. P. 121-130.

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

Synergistic Activities

2018 Origins Fellow at Case Western Reserve University
2016-2018 500 Women Scientists Outreach in Knoxville, TN

Collaborators & Other Affiliations

Collaborators

J. Bartley, Department of Geology, Gustavus Adolphus College; T. Selly, Department of Geology, University of Missouri; K. Williford, Planetary Geochemistry, The NASA Jet Propulsion Laboratory; M. Tuite, Planetary Geochemistry, The NASA Jet Propulsion Laboratory; R.S. Wood, Department of Geology, Washington University; J. Dunham, Bureau Veritas; E. Goodman, Hess Corporation

Graduate Advisor

Linda Kah, Department of Earth and Planetary Sciences, University of Tennessee at Knoxville

Research Impacts

Established new methodologies for sample preparation when working with rare/limited sample sizes such as those coming back from a Mars mission.

Biographical Sketch for Eleni Panagiotou

(tenure-track) Assistant Professor Department of Mathematics, University of Tennessee at Chattanooga, TN 37403 805-6373313 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
Programme Participant, Isaac Newton Institute for the Mathematical Sciences, Cambridge, UK, 2012
Visiting Researcher, Swiss Federal Institute of Technology ETH Zurich, 2011–2012

Publications, related to the current project

1. Panagiotou E. and Plaxco, W. K., 2018, A topological study of protein folding kinetics (submitted)

2. Panagiotou E., Millett K. C. and Atzberger P., 2017, Topological Methods for Polymeric Materials: Characterizing the Relationship Between Polymer Entanglement and Viscoelasticity, (submitted). [link to preprint]

3. Panagiotou E. 2015, The linking number in systems with periodic boundary conditions, *J. Comp. Phys.* **300** 533-573.[link to full paper]

4. Panagiotou E. and Kröger M., 2014, Pulling force-induced elongation and alignment effects on entanglement and knotting characteristics of linear polymers in a melt *Phys. Rev. E* **90** 042602.[link to full paper]

5. Panagiotou E., Kröger M and Millett K. C., 2013, Writhe and mutual entanglement combine to give the entanglement length *Phys. Rev. E* **88** 062604.[link to full paper]

Publications, other

1. Panagiotou E. and Millett K. C., 2018, Linking matrices in systems with periodic boundary conditions J. Phys. A: Math. Theor. [link to preprint]

2. Millett K. C. and Panagiotou E., 2016, Entanglement transitions in one dimensional confined flows, *Fluid dynamics Research* (accepted manuscript).[link to preprint]

3. Igram S., Millett K. C. and Panagiotou E., 2016, Resolving critical degrees of entanglement in olympic rings systems, *J. Knot Theory Ramif.* **25** 14.[link to full paper]

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

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

Synergistic Activities

1. 2014 Co-supervision of senior thesis of Spencer Igram, STEM student, UCSB

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 and "The linking number in systems of curves with Periodic Boundary Conditions", Invited talk to SIAM Undergraduate Research Mini-symposium, University of California, Santa Barbara, May 2014

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Assistant Professor
615 McCallie Ave, Chattanooga, TN 37403
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(a) Professional Preparation

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

(b) Appointments

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

(c) Publications

Pienkos, J. A.; Webster, A. B.; Piechota, E. J.; Agakidou, A. D.; McMillen, C. D.; Pritchett, D. Y.; Meyer, G. J.; Wagenknecht, P. S. Oxidatively stable ferrocenyl-π-bridge-titanocene D-π-A Complexes: an electrochemical and spectroscopic investigation of the mixed-valent states. *Dalton Transactions* **2018**, 47, 10953.

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

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

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

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

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

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

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

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

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

(d) Synergistic Activities

- Helped organize science workshops for local high school students and teachers (2015-present).
- Organized three guest lectures at Furman University (2016-2017)
- Organized two guest lectures at University of Virginia (2012-2013)
- University of Virginia Chemistry Graduate Student Council (2010-2013)
- Developing outreach activities which utilize the WebMO computational chemistry program.

Biographical Sketch

Hong Qin

University of Tennessee at Chattanooga
Department of Computer Science & Engineering
Department of Biology, Geology & Environmental Science, SimCenter
Phone: 423-425-4329 Fax: 423-425-5442 Email: hong-qin@utc.edu

a. Professional Preparation

- Tsinghua University, China, Biological Sciences and Biotechnology, B.S, 1991
- Tsinghua University, China, Biophysics, M.S.,1994
- University of Chicago, Biochemistry and Molecular Biology, Ph.D, 2000
- Loyola University of Chicago, Computer Science, M.S., 2002

b. Appointments

- Associate Professor, joint appointment in Department of Computer Science & Engineering and Department of Biology, Geology & Environmental Science, and SimCenter, August 2016 – present.
- Adjunct Associate Professor, College of Medicine Chattanooga, University of Tennessee Health Science Center, October 2017 – present.
- Associate Professor, Department of Biology, Spelman College, September 2015 – July 2016.
- Assistant Professor, Department of Biology, Spelman College, August 2009 – August 2015.
- Assistant Professor, Department of Agricultural and Environmental Sciences, and Department of Biology, Tuskegee University, February 2007 – July 2009.
- Research Assistant Professor, Department of Biostatistics and Computational Biology, Center for Aging and Development Biology, University of Rochester. January 2004- June 2006

c. Publications (10 out 21) *Asterisks indicate undergraduate co-authors*

i) Five publications most closely related to proposed project:

- Guven, E., H. Qin, The effect of Gaussian noise on maximum likelihood fitting of Gompertz and Weibull mortality models with yeast lifespan data. Experimental Aging Research. Accepted.
- Guven, E., L.A. Parnell*, E.D. Jackson*, M.C. Parker*, N. Gupta, J. Rodrigues, and H. Qin, Hydrogen peroxide induced loss of heterozygosity correlates with replicative lifespan and mitotic asymmetry in Saccharomyces cerevisiae. PeerJ, 2016. 4: p. e2671
- Jiang, Y., H. Qin, and L. Yang, *Using network clustering to predict copy number variations associated with health disparities.* PeerJ, 2015. 3: p. e677.4358638.
- Qin, H. and A. Driks, *Contrasting evolutionary patterns of spore coat proteins in two Bacillus species groups are linked to a difference in cellular structure.* BMC Evol Biol, 2013. 13(1): p. 261.
- Qin, H., *Teaching computational thinking through bioinformatics to biology students.* Proceedings of 40th ACM Technical Symposium on Computer Science Education, 2009: p. 188-191.

ii) Five other significant publications:

- Guo, Z., A.B. Adomas, E.D. Jackson*, H. Qin, and J.P. Townsend, *SIR2 and other genes are abundantly expressed in long-lived natural segregants for replicative aging of the budding yeast Saccharomyces cerevisiae.* FEMS Yeast Res, 2011. **11**(4): p. 345-55.

- Qin, H., M. Lu, and D.S. Goldfarb, *Genomic instability is associated with natural life span variation in Saccharomyces cerevisiae.* PLoS ONE, 2008. **3**(7): p. e2670.
- Qin, H., H.H. Lu, W.B. Wu, and W.H. Li, *Evolution of the yeast protein interaction network.* Proc Natl Acad Sci U S A, 2003. **100**(22): p. 12820-4.
- Gilchrist, M.A., H. Qin, and R. Zaretzki, *Modeling SAGE tag formation and its effects on data interpretation within a Bayesian framework.* BMC Bioinformatics, 2007. **8**: p. 403.
- Qin, H., W.B. Wu, J.M. Comeron, M. Kreitman, and W.H. Li, *Intragenic spatial patterns of codon usage bias in prokaryotic and eukaryotic genomes.* Genetics, 2004. **168**(4): p. 2245-60.

d. Synergistic Activities

- **NSF CAREER award** #1453078, "A probabilistic gene network model of cellular aging and its application on the conserved lifespan extension mechanisms of dietary restriction." Dr. Qin is the recipient of an NSF CAREER award for his research on mathematical modeling of cellular aging and development of computational tools for studies on aging.
- **"Video Genomics Working Group"** and **Faculty Mentor Fellow of Quantitative Undergraduate Biology Education and Synthesis (QUBES)**: Dr. Qin is an inaugural member of the QUBES Faculty Mentor Fellow Program in 2017. Dr. Qin led an online faculty workshop on developing video tutorials of computational genomics into undergraduate interdisciplinary education and research.
- **Support for under-represented groups in STEM**. Qin provide support of computational analysis and advice to colleagues at Spelman College, Tuskegee University, and Norfolk State University. Qin is participating in an NSF funded scholarship program ASPIRE for STEM students from low-income families at UTC. Qin is the 2016 recipient of the William A. Hinton Research Training Award from the American Society for Microbiology, based on his records of engaging under-represented minority students in his research.
- **Quantitative Biology Community**: Qin maintains the http://compmodelmatch.org website for the workshop series, "Finding your inner modeler: how computational biology can advance your research and how to get started," supported by an NSF MCB award (PI David Stone, U of Illinois at Chicago). Qin also recently co-organized the NSF-sponsored workshop, "A strategic planning workshop to explore quantitative biology as a vehicle for broad participation" (see https://youtu.be/eoQ0VXcSimg).
- **YouTube Educational Channel**, http://youtube.com/c/hongqin. Dr. Qin has been developing educational and tutorial videos since 2009. His educational channel covers computational biology, molecular biology, and microbiology. His educational channel has over 500 subscribers and over 250,000 views. Dr. Qin's popular education videos include: "Visualizing protein structure in Swiss PDB Viewer," "How to use R match() function to merge different data sets," "Retrieve and analyze a gene expression data set from NCBI GEO in R," "Covert Excel file to csv and read into R," "Principle of site-directed mutagenesis by PCR," "BD FACS Calibur, Cell Quest Training," "Hierarchical clustering by hclust in R on a distance matrix," and "PCR product analysis followed by restriction enzyme analysis, ApE."

Reetesh Ranjan
Research Engineer II
School of Aerospace Engineering
Georgia Institute of Technology
270 Ferst Dr NW, Atlanta
GA 30332
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(a) Professional Preparation

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

(b) Appointments

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

(c) Products

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

(ii) Ranjan, R., Menon, S., & Munipalli, R. (2018). Reduced Basis Modeling of Single-Element Subscale Rocket Combustors. In *2018 Joint Propulsion Conference* (p. 4871). https://doi.org/10.2514/6.2018-4871

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

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

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

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

(vii) Ranjan, R., & Menon, S. (2018). Vorticity, backscatter and counter-gradient transport predictions using two-level simulation of turbulent flows. *Journal of Turbulence*, *19*(4), 334-364. https://doi.org/10.1080/14685248.2018.1438616

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

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

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

(d) Synergistic Activities

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

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

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

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

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

PI: Mina Sartipi, PhD

UC Foundation Professor - Department of Computer Science and Engineering
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The University of Tennessee at Chattanooga
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A. Professional Preparation

Sharif University of Technology	Tehran, Iran	Electrical Engineering	B.Sc., 2000
Georgia Institute of Technology	Atlanta, GA	Electrical and Computer Eng.	M.S., 2003
Georgia Institute of Technology	Atlanta, GA	Electrical and Computer Eng.	Ph.D., 2006

B. Appointments

2018–present **Founding Director**
Center for Urban Informatics and Progress (CUIP)
University of Tennessee at Chattanooga,
Chattanooga, TN, USA

2017–present **Faculty Member**
Bredesen Center for Interdisciplinary Research and Graduate Education
University of Tennessee Knoxville,
Knoxville, TN, USA

2016–present **Lead Scientist Smart City and Urban Systems**
University of Tennessee at Chattanooga,
Chattanooga, TN, USA

2015–present **Professor & PhD Program Coordinator**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering,
Chattanooga, TN, USA

2011–2015 **Associate Professor**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering
Chattanooga, TN, USA

2007–2011 **Assistant Professor**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering
Chattanooga, TN, USA

2006–2007 **Assistant Professor**
University of Tennessee at Chattanooga, Dept. of Electrical Engineering
Chattanooga, TN, USA

C. Products

Products Most Closely Related to Proposal

[1] R. Thompson, Z. Hu, J. Cho, J. Stovall, A. Harris, and M. Sartipi, "Enhancing Driver Awareness Using See-Through Technology." WCX17: SAE World Congress Experience, 2017.

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

[3] National Science Foundation NSF – Lead PI: *US Ignite: Collaborative Research: Focus Area 1: Fleet Management of Large-Scale Connected and Autonomous Vehicles in Urban Settings* (in collaboration with Dr. Samoylov and Dr. McMurray, Georgia Tech Institute of

Technology), January 2017.

[4] M. Sartipi and R. Thompson, "Real-Time See Through Technology for Collected Autonomous Vehicles," US Ignite Application Summit and Smart Cities Connect Conference, Live Demonstration, June 2017.

[5] J. Cho, Z. Hu, and M. Sartipi, "Non-Intrusive A/C Load Disaggregation Using Deep Learning," accepted to appear in the Proc. of 2018 IEEE Power & Energy Society T&D Conference & Exposition, April 2018.

Other Significant Products

[1] B. Williams, B. Allen, Z. Hu, H. True, J. Cho, A. Harris, N. Fell, and M. Sartipi, "Real-Time Fall Risk Assessment Using Functional Reach Test," The International Journal of Telemedicine and Applications, January 2017.

[2] Z. Hu, S. Mohagheghi, and M. Sartipi, "Flexible Data Acquisition, Compression, and Reconstruction in Advanced Metering Infrastructure", in Proc. of Power Systems Conference, March 2016.

[3] J. Cho, Z. Hu, and M. Sartipi, "Post-stroke Discharge Disposition Prediction using Deep Learning," in Proc. of IEEE SoutheastCon, March 2017.

[4] M. Sartipi, "Low-Complexity Distributed Compression in Wireless Sensor Networks", in Proc. IEEE Data Compression Conference, March 2012.

[5] M. Sartipi, F. Fekri, "Distributed Source Coding using Short to Moderate Rate-Compatible LDPC Codes: The Entire Slepian-Wolf Rate Region," IEEE Transactions on Communications, Volume 56, Issue 3, pp. 400-411, March 2008.

D. Synergistic Activities

- **IEEE Senior Member**
- **NSF Panelist -** 2009 - present
- **Member of the board of directors**

  Chattanooga Enterprise Center, April 2017-present

  Variable Inc, 2012-present
- **Faculty Advisor -** 2016-present, Girls in Computer Science (GiCS)
- **Award**
  - o UTC Outstanding Faculty Research and Creative Achievement award, 2016
  - o "Keep the Stars Shining" Award, 2012
  - o Outstanding Researcher in the College of Engineering and Computer Science, 2010, 2014, 2015
  - o Outstanding Researcher in the Department of Computer Science and Engineering, 2010, 2013, 2015
  - o Named UC Foundation Assistant Professor, 2008

Jin Wang

Professor and UNUM Chair of Excellence
Department of Mathematics
University of Tennessee at Chattanooga

Professional Preparation

University of Science & Technology of China	Mathematics	B.S.	(1994-1998)
University of Science & Technology of China	Mathematics	M.S.	(1998-2000)
The Ohio State University (Columbus, OH)	Mathematics	Ph.D.	(2000-2004)

Appointments

2014-present	University of Tennessee at Chattanooga	Professor
2012-2014	Old Dominion University	Associate Professor
2007-2012	Old Dominion University	Assistant Professor
2005-2007	Duke University	Assistant Research Professor
2004-2005	The Ohio State University	Lecturer

Publications (related to the proposed project)

1. F. Bao, L. Mu and **J. Wang**, A fully computable posteriori error estimate for the Stokes equations on polytopal meshes, *SIAM Journal on Numerical Analysis*, 2018. Accepted.

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

3. A. Timalsina, J. Tian and **J. Wang**, Mathematical and computational modeling of tumor virotherapy with mediated immunity, *Bulletin of Mathematical Biology*, vol. 79, pp. 1736-1758, 2017.

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

5. **J. Wang**, C. Modnak and G. Hou, Convergence analysis of an iterative algorithm for a class of constrained dynamic problems, *Applied Mathematics and Computation*, vol. 219, pp. 1200-1221, 2012.

6. G. Hou, **J. Wang** and A. Layton, Numerical methods for fluid-structure interaction - A review, *Communications in Computational Physics*, vol. 12(2), pp. 337-377, 2012.

7. **J. Wang** and A. Layton, Numerical simulations of fiber sedimentation in Navier-Stokes flows, *Communications in Computational Physics*, vol. 5(1), pp. 61-83, 2009.

8. **J. Wang** and G. Baker, A numerical algorithm for viscous incompressible interfacial flows, *Journal of Computational Physics*, vol. 228, pp. 5470-5489, 2009.

9. **J. Wang**, An asymptotic expansion for Stokes waves with viscosity, *Fluid Dynamics Research*, vol. 40, pp. 155-161, 2008.

10. **J. Wang**, Computation of 2D Navier-Stokes equations with moving interfaces by using GMRES, *International Journal for Numerical Methods in Fluids*, vol. 54, pp. 333-352, 2007.

Synergistic Activities

- Reviewer: *Journal peer review (more than 70 manuscripts in 38 journals); Grant panel/review (National Science Foundation, National Institutes of Health, Kentucky Science & Engineering Foundation, Georgian National Science Foundation, etc.); Conference proceedings review (more than 10 conferences); Book review (4 books).*

- Organizer: *Minisymposium on "Simulation and Analysis in Biological Systems", the 35th SIAM-SEAS Conference, Charlotte, NC, March 2011; Minisymposium on "Recent Advances in Mathematical Epidemiology and Ecology", The 4th International Conference on Mathematical Modeling and Analysis, Lubbock, TX, October 2013; International Conference on "Recent Advances in Linear Algebra and Graph Theory", Chattanooga, TN, March 2016; Interdisciplinary Mathematics Summer Camp for High School Students, Chattanooga, TN, 2016, 2017, 2018; Workshop on "Epidemic Dynamics of Cholera in Non-homogeneous Environments", American Institute of Mathematics, San Jose, CA, July 2016.*

- Grant activity: *Nearly 2.5 million of research grants from federal, state and private funding agencies during the last 10 years, including 7 grants from the National Science Foundation.*

- University service: *Curriculum Committee (2009, 2015, 2016), Colloquium Committee (2014-2018), Faculty Search Committee (2009-2010, 2014-2018), Tenure and Promotion Committee (2015-2018), Computational Science Ph.D. Screening Committee (2016-2017), Doctoral Dissertation Committees (Fernando, 2008; Brown, 2010; Neamprem, 2010; Liao, 2010; Malali, 2012; Modnak, 2013; Posny, 2014; Gounley, 2014; Ghazizadeh, 2014; Malali, 2015; Timalsina, 2017; Edwards, 2017; Trimble, 2018), Qualifying Examination Committees (Li, Posny, Phuworawong, 2011; Malali, 2012; Ghazizadeh, 2013; Trimble, 2017; Altarawneh, Dai, Ghafari, Omwenga, Phuong, Saied, Schwab, 2018).*

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

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518 Oak St.
Chattanooga, TN 37403
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423-425-5394

(a) Professional Preparation

Eastern Kentucky University	Richmond, KY	Athletic Training	BS, 1978
University of Arizona	Tuscon, AZ	Athletic Training	MS, 1979
University of Kentucky	Lexington, KY	Education-Kinesiology	EdD, 1989

(b) Appointments

1999-	Tenured Professor, University of Tennessee at Chattanooga, Chattanooga, TN
1994-1999	Co-Founder and CEO, BioKinetics Therapy & Training, Inc., Paducah, KY
1991-1994	Director of Sports Medicine Research & Education, Trover Clinic, Madisonville, KY
1980-1991	Head Athletic Trainer and Biology Instructor, Centre College, Danville, KY
1979-1980	Head Athletic Trainer, Amphitheater High School, Tucson, AZ

(c) Publications

Wilkerson GB, Nabhan DC, Prusmack CJ, Moreau WJ. Detection of persisting concussion effects on neuromechanical responsiveness. *Med Sci Sports Exer*. 2018;50(9):1750-1756. PMID:29683918.

Wilkerson GB, Grooms DR, Acocello SN. Neuromechanical considerations for postconcussion musculoskeletal injury risk management. *Curr Sports Med Rep*. 2017;16(6):419-427. PMID:29135640.

Wilkerson GB, Simpson KA, Clark RA. Potential for improvement of visuomotor reaction time among college football players. *J Sport Rehabil.* 2017;26(1):26-34. PMID:26797726.

Wilkerson GB, Colston MA. Refinement of a prediction model for the occurrence of core and lower extremity sprains and strains in college football players. *J Athl Train*. 2015;50(6):643-650. PMID:25844856.

Wilkerson GB, Gupta A, Allen JR, Keith CM, Colston MA. Utilization of inertial measurement unit data for quantification of college football injury risk. *J Strength CondRes.* 2016;30(9):2369–2374. PMID:26849792.

(d) Synergistic Activities

Editor-in-Chief, *International Journal of Athletic Therapy & Trianing*, 2003-2013

Board of Advisors, Secondary School Athletic Training Practice-Based Research Network, 2010-2018

Scientific Advisory Board, Datalys Center NCAA Injury Surveillance System, 2010-2018

Institutional Review Board Member, University of Tennessee Chattanooga, 2002-2018

Atlanta Olympic Games Sports Medicine Staff, Olympic Village Polyclinic, 1996

Dalei Wu, PhD

Assistant Professor
Department of Computer Science and Engineering
The University of Tennessee at Chattanooga
Phone: (423) 425-4386, Fax: (423) 425-5442
Email: dalei-wu@utc.edu

A. Professional Preparation

Shandong University	Jinan, China	Electrical Engineering	B.Sc., 2001
Shandong University	Jinan, China	Electrical Engineering	M.S., 2004
Univ. of Nebraska-Lincoln	Lincoln, USA	Computer Engineering	Ph.D., 2010
Massachusetts Institute of Tech.	Cambridge, USA	Postdoc, Mechatronics	11/2011-06/2014

B. Appointments

2014–present **Assistant Professor**
University of Tennessee at Chattanooga, Dept. of Computer Science and Engineering, Chattanooga, TN, USA

2004–2005 **System Engineer**
ZTE Telecom Corporation, WiMAX R&D, Shenzhen, China

C. Publications

Publications most closely related to proposed project

[1] S. Guo and D. Wu and H. Zhang and D. Yuan, "Resource Modeling and Scheduling for Mobile Edge Computing: A Service Provider's Perspective," *IEEE Access*, vol. 2018.

[2] D. Wu, D. Chatzigeorgiou, K. Youcef-Toumi, and R. Mansour, "Node Localization in Robotic Sensor Networks for Pipeline Inspection," *IEEE Transactions on Industrial Informatics*, vol. 12, no. 2, April, 2016.

[3] D. Wu, Q. Liu, H. Wang, D. Wu, and R. Wang, "Socially-Aware Energy-Efficient Mobile Edge Collaboration for Video Distribution," *IEEE Transactions on Multimedia*, vol. 19, no. 10, Oct. 2017.

[4] D. Wu, J. Yan, H. Wang, D. Wu, and R. Wang, "Social Attribute Aware Incentive Mechanism for Device-to-Device Video Distribution," *IEEE Transactions on Multimedia*, vol. 19, no. 8, Aug. 2017.

[5] D. Wu, S. Ci, H. Luo, Y. Ye, and H. Wang "Video Surveillance over Wireless Sensor and Actuator Networks Using Active Cameras," *IEEE Transactions on Automatic Control*, vol. 56, no. 10, Oct. 2011.

Other significant publications

[1] D. Wu, S. Ci, H. Luo, and H. Guo, "A Theoretical Framework for Interaction Measure and Sensitivity Analysis in Cross-Layer Design," *ACM Transactions on Modeling and Computer Simulation*, vol. 21, issue 1, Dec. 2010.

[2] D. Wu, D. Chatzigeorgiou, K. Youcef-Toumi, S. Mekid, and R. Mansour, "Channel-Aware Relay Node Placement in Wireless Sensor Networks for Pipeline Inspection," *IEEE Transactions on Wireless Communications*, vol. 13, no. 7, July, 2013.

[3] D. Wu, S. Ci, H. Wang, and A. Katsaggelos, "Application-Centric Routing for Video Streaming over Multi-hop Wireless Networks", *IEEE Transactions on Circuits and Systems for Video Technology*, vol. 20, no. 12, Dec. 2010.
[4] Dalei Wu, Song Ci, and Haohong Wang, "Cross-Layer Optimization for Video Summary Transmission over Wireless Networks", *IEEE Journal on Selected Areas in Communications*, vol. 25, no. 4, May 2007, pp. 841-850.
[5] S. Guo, H. Zhang, P. Zhang, D. Wu, and D. Yuan, "Generalized 3-D Constellation Design for Spatial Modulation," *IEEE Transactions on Communications*, vol. 65, no. 8, Aug. 2017.

D. Synergistic Activities

- PI at UTC for the project NSF US Ignite: Collaborative Research: Focus Area 1: Fiber Network for Mapping, Monitoring and Managing Underground Urban Infrastructure," Award No. 1647175, $299,884, 01/2017 – 12/2019. Through collaboration between UTC and University of Vermont as well as interaction with utility engineers, managers and city officials, the project involves fundamental research on network-enabled underground infrastructure sensing and information processing, most of which has not yet been done on a citywide scale. In this project, Dr. Wu has involved one female graduate to the completion of her master degree, one graduate pursuing his Ph.D. degree, and several undergraduates in conducting the related research to solve real-world problems and benefit city and community.

- UTC Undergraduate Research and Creative Endeavor (URaCE) Summer Fellowship in Smart Cities and Urban Systems, $15,000, 05/2018 - 08/2018, PI for the project "Developing an Edge Computing Platform for Urban Augmented Reality Applications." Dr. Wu involved three undergraduate students (two in computer science and one in mathematics) in research on developing an edge computing platform for computation-intensive and latency-sensitive augmented reality applications in the summer of 2018.

- Participation in GIGTANK – an immersive 12-week experience for startups developing business applications that thrive on low latency networks. Dr. Wu formed a team consisting of undergraduates and faculty to participate in the training for developing a startup focused on underground infrastructure mapping based on gigabit Internet, in Chattanooga, TN, the home of America's largest ubiquitous fiber network. With the guidance of industry experts, the team acquired experience in product development, business model invention, and go-to-market strategy in the hyper-connected world.

- Mentor of the FIRST Robotics Competition (FRC), Chattanooga Girls Leadership Academy, 12/2017. In this activity, Dr. Wu taught high school girls the basics of sensors, motion control, and wireless communications. He also served as a judge of the First Lego League Robotics Competition for middle schools, Red Bank Middle School.

- Participation in training high school teachers as part of the Hamilton County schools Future Ready Institute initiative in 06/2018. As part the training activities, Dr. Wu gave presentation and hands-on lab in using deep learning for data analytics.

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
Postdoctoral	MIT	Mechanical Engineering	2012 – 2014

(b) Appointments

2017 – Present	University of Tennessee at Chattanooga, Assistant Professor
2015 – 2017	MIT, Research Scientist

(c) Products

(i) Most Closely Related Products

1. H. Kim, S. Yang, S. Narayanan, H. Furukawa, J. Jiang, A. Umans, O. Yaghi and E. Wang, Harvesting Water from Humid Air using Metal-Organic Frameworks, Science 356, 6336, 430-434 (2017)
2. H Kim, SR Rao, EA Kapustin, L Zhao, S Yang, OM Yaghi, EN Wang, Adsorption-based atmospheric water harvesting device for arid climates, Nature communications 9 (1), 1191 (2018)
3. Yang, S., Huang, X., Chen, G. et al. Three-dimensional graphene enhanced heat conduction of porous crystals, *J Porous Mater* (2016) 23: 1647
4. 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. S. Narayanan, H. Kim, A. Umans, S. Yang, X. Li, S. Schiffres, S. Rao, C. Rios, C. Hidrovo, and E. Wang, A Thermophysical Battery for Storage-based Climate Control, Applied Energy, 189, 1, 31–43 (2017)

(ii) Other Products

1. A Rieth, S Yang, E Wang, M Dinca, Record Atmospheric Fresh Water Capture and Heat Transfer with a Material Operating at the Water Uptake Reversibility Limit, ACS Cent. Sci., 3 (6), pp 668–672 (2017)
2. H. Kim, H. J. Cho, S. Narayanan, S. Yang, S. Schiffres, X. Li, H. Furukawa, Y. Zhang, J. Jiang, O. M. Yaghi and E. N. Wang, Characterization of Adsorption Enthalpy of Novel Water-Stable Zeolites and Metal-Organic-Frameworks, Scientific Reports, 2016, 6, 19097
3. S. Narayanan, X. Li, S. Yang, H. Kim, A. Umans, I.S. McKay, E.N. Wang, Thermal battery for portable climate control, Applied Energy, 149, 104-116, 2015.
4. S. Narayanan, S. Yang, H. Kim, and E. Wang, Optimization of Adsorption Processes for Climate Control and Thermal Energy Storage, Journal of heat transfer, 2014, 77, 288–300.
5. LA Weinstein, K McEnaney, E Strobach, S Yang, Hybrid Electric and Thermal Solar Receiver, *Joule*, 2 (5) 2017, 962-975A

(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.

Biographical Sketch

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

(a) Professional Preparation

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

(b) Appointments

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

(c) Products

(i) Five Relevant Products

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

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

Yang, W.-Y.; Wilson, H. D.; Velagapudi, S. P.; Disney, M. D. **Covalent small molecule targeting of r(CGG)^{exp} inhibits non-ATG-initiated translation in FXTAS.** *J. Am. Chem. Soc.* **2015, *137,* 5336**

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

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

(ii) Five Other Significant Publications

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

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

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

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

Haga, C. L.; Velagapudi, S. P.; Strivelli, J.; Yang, W.-Y.; Disney, M. D.; Phinney, D. G. **Small Molecule Inhibition of miR-544 Biogenesis Disrupts Adaptive Responses to Hypoxia by Modulating ATM-mTOR Signaling.** *ACS Chem. Biol.* **2015**, *10*, 2267

(d) Synergistic Activities

1) Interdisciplinary projects

2) Mentoring 13 Undergraduate Students in Research Program (2007-2011)

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

3) Member of the Inter-American Photochemical Society (2007-2008)

Appendix B

Awardee Project Reports

New Projects for FY 2020

Fiscal Year 2020 Final Project Report

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

Dr. Bradley J. Harris, Lead PI

Co-PI(s): Dr. David Giles
Other Personnel: Andrew Turgeson, Graduate Research Assistant; Konner Glass, Undergraduate Research Assistant; Devin Martin, Undergraduate Research Assistant; Diane Madeksho, Undergraduate Research Assistant; Dalton Strike, Undergraduate Research Assistant; Christopher Dowell, HPC Administrator

Project Title: The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence

Date Submitted: 7/30/2020

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

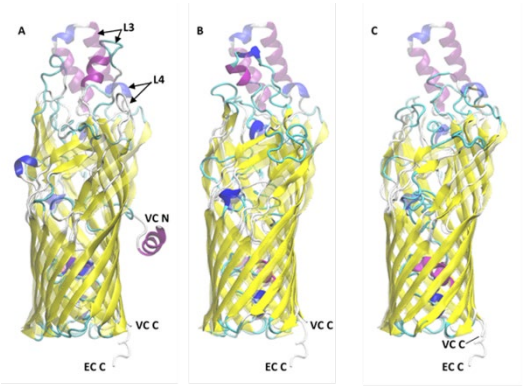
Non-Technical Summary:

Antibiotic-resistant pathogens represent an escalating threat to public health worldwide, and rising rates of resistance among Gram-negative bacteria are of particular concern. These bacteria have evolved a number of endogenous membrane remodeling strategies to sense and adapt to their environment. However, another membrane remodeling strategy employed by these bacteria, the uptake and assimilation of exogenous fatty acids into membrane phospholipids, remains largely unexplored. The proposed project aimed to enhance our scientific understanding of how fatty acid uptake contributes to the pathogenicity and virulence of Gram-negative pathogens through experimentally-guided simulation. The major objectives of the project were to: (1) determine the impact of phospholipid remodeling on virulence phenotypes in the model organism *Vibrio cholerae* (or *Vc*); (2) identify the effects of fatty acid assimilation on *Vc* membrane behavior; and (3) determine the role of fatty acid transporter homologs in the recognition of exogenous fatty acids in *Vc*.

Key findings include preliminary data that suggests phospholipid remodeling through the assimilation of free fatty acids impacts antimicrobial resistance in *Vc*, as well as structural modeling data that reveals structural differences in fatty acid transporter homologs in *Vc* that could have crucial implications for pathogenicity. Key outcomes include the submission of a conference paper to the AIChE 2020 annual conference (accepted), the pending submission of two journal articles, and submission of a NSF CAREER proposal. Student impacts included support of three undergraduate chemical engineering students (including one DHON thesis), as well as one Ph.D. computational engineering student. This project advanced the mission of the SimCenter by mentoring students and providing seed funding for applied computational science in health and biological systems.

PROJECT TITLE: The Impact of Membrane Phospholipid Remodeling on Pathogen Survival and Persistence

Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
This project aimed to quantify the extent to which free fatty acids (FFAs) contribute to pathogenicity and virulence in Gram-negative bacteria, and determine the molecular mechanisms by which FFA recognition is accomplished. • Determine the impact of phospholipid (PL) remodeling on virulence in the model organism *Vibrio cholerae* (or *Vc*); • Identify the effects of fatty acid assimilation on *Vc* membrane behavior; • Determine the role of fatty acid transporter homologs in the recognition of exogenous fatty acids in *Vc*.	Key findings include: • Preliminary data suggests PL remodeling through the assimilation of FFAs impacts antimicrobial resistance in *Vc*; • Structural modeling reveals differences in fatty acid transporter homologs in *Vc* that could have crucial implications for pathogenicity Key outcomes include: • Submission of a conference paper to AIChE 2020 annual conference (abstract accepted) • Submission of a NSF CAREER proposal • Two manuscripts in preparation
RESULTS	**OTHER INFO**
 **Figure 1.** Superposition of *E. coli* crystal structure (transparent) onto the *V. cholerae* (opaque) homology models (A) NP_230687, (B) NP_230688, and (C) NP_233248. Visually discernible differences include the L3/L4 loops, the N terminus hatch domain, and the location of the C terminus (EC C versus VC C).	**Budget and Schedule** Total Budget: $92,742.00 Actual Used: $89,706.71 Balance: $11,235.29 Total period of performance is 12 months. Task 1: Months 1-9 Task 2: Months 1-8 Task 3: Months 9-12 **Deliverables** • Quarterly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication • External and internal conference presentation

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Experimental assessment of impact of PL remodeling on *Vc* antimicrobial resistance	Recruited and trained ugrad student researchers and optimized antimicrobial resistance assay; developed list of target LPS-deficient strains from Co-PI Giles mutant library and acquired human gut- and fish-specific antimicrobial peptides from appropriate vendors; conducted antimicrobial resistance assays, analyzed and interpreted data
Computational modeling of *Vc* outer membrane	Recruited and trained Ph.D. student researcher; constructed Vc-specific LPS molecule and created outer membrane model; conducted membrane model simulations, analyzed and interpreted data
Computational modeling of *Vc* fatty acid transporter homologs	Trained Ph.D. student researcher; identified three most prevalent fatty acid transporter homologs in *Vc*; predicted three-dimensional structures using homology modeling; identified structural differences in key FFA binding sites
Disseminate research at local, regional, and national conferences, as well as via peer-reviewed publications	ASM Microbe 2020 (poster abstract accepted but conference postponed); AIChE 2020 annual conference (conference paper abstract accepted)
Submit external grant proposals utilizing preliminary data collected	NSF CAREER proposal for PI Harris submitted July 2020
Disseminate research via peer-reviewed publications	Two manuscripts currently in preparation

Challenges & Strategies Used to Address / Overcome:

Challenge #1: Initial results utilizing a microtiter-plate based assay to quantify antimicrobial resistance were inconsistent. Strategy Used to Overcome: Worked with DHON and co-PI Giles to develop alternative CFU-based assay.

Challenge #2: Encountered numerous difficulties when attempting to build outer membrane bilayers solely from in-house code (e.g., naming convention issues, atom overlaps, non-converging simulations). Strategy Used to Overcome: Worked with Ph.D. student to identify CHARMM-GUI, an online simulation input generator well-cited in the literature, and developed in-house code to handle exotic UFAs not available in online database.

Challenge #3: No discernible trends in outer membrane modeling data after thorough review. Strategy Used to Overcome: Shifted focus to homology modeling of fatty acid transport system in Vc. Trained Ph.D. student on use of NCBI BLAST and I-TASSER.

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

Our strategy for using molecular dynamics to study the impact of phospholipid remodeling on membrane function in *Vc* ultimately yielded no useful results. The PI had been contemplating the use of structural modeling to study the differences in long-chain fatty acid transporters in *Vc*, as prior research shows that it possesses more genetic copies compared to other bacteria and this could be important for its ability to cycle between environments. With a competent and motivated Ph.D. student available to undertake the task, the research team elected to shift focus. This resulted in key preliminary data that supports one of the specific aims in the PI's recently submitted NSF CAREER proposal.

IMPACT & OUTCOMES

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

The preliminary data and evidence of prior collaboration enabled by this and prior CEACSE awards were key in securing our recent NIH R15 award #1R15GM131315-01A1, on which Drs. Harris and Giles are co-Investigators with PI Dr. Jin Wang. The current CEACSE award also provided critical preliminary data for the NSF CAREER proposal recently submitted by PI Harris.

Students Impacted

Konner Glass, seeking B.S. ChE. Gained valuable experience in experimental design and execution, and presented research at local conferences.

Devin Martin, seeking B.S. ChE. Gained valuable experience in experimental design and execution, as well as literature review and manuscript preparation.

Diane Madeksho, seeking B.S.Chemistry. Gained valuable experience in literature review and manuscript preparation.

Dalton Strike, B.S. ChE Spring 2020. Gained valuable experience in experimental design and execution, functioned as research team lead through training and mentoring of fellow ugrad students, and presented research at numerous local, regional, and national conferences. This research was also the focus of his DHON thesis.

Andrew Turgeson, seeking Ph.D. in Computational Engineering. Gained valuable experience in computational modeling and structural analysis of biomacromolecules, as well as literature review and manuscript preparation.

Community and Broader Impacts

Our contribution here is expected to enhance understanding of the fatty acid assimilation capabilities of Gram-negative pathogens and their impact on pathogenicity and virulence. This contribution is significant because it is expected to be of translational importance in the prevention and treatment of diseases caused by pathogens with fatty acid uptake ability. Successful completion of this work is expected to inform subsequent studies that will focus on bacterial interactions with microbiota present in environmental reservoirs. This progression of research is expected to significantly enhance our understanding of microbial ecology and addresses two of the long-term bold research goals identified by NSF in its "10 Big Ideas for

NSF Future Investments". Specifically, this research seeks to better understand the interactions between microbe, host, and environment and approach scientific inquiry in a way that crosses scales and disciplines (Understanding the Rules of Life). Furthermore, this research identifies a complex grand challenge (human health) and aims to merge the ideas, approaches, and technologies of engineering and biology in order to address it (Growing Convergence Research).

Furthermore, the submitted NSF CAREER proposal couples this research with a strong educational outreach aim focused on improving learning outcomes for engineering transfer students. As such, the proposed education plan is expected to have a significant positive societal impact. Namely, this project is expected to result in improved STEM education and educator development. In addition, the CCs collaborating on the project serve a student population that is largely minority, first-generation, low-income, and adult students. Consequently, this project will contribute to the development of a diverse, globally competitive STEM workforce.

Scholarly Products

External Conferences:

1. Strike, W., Martin, D., Glass, K., Harris, B. Phospholipid remodeling via exogenous polyunsaturated fatty acid uptake modulates stress resistance in Vibrio cholerae. Poster presented at: AIChE National Conference; 2019 November 11; Orlando, FL.
2. Rojas, E., Giles, D., Wang, J., and Harris, B. Influence of population density and environmental conditions on *V. cholerae* growth and virulence. ASM Microbe 2020 June 18-22; Chicago, IL (abstract accepted for poster presentation, conference postponed).
3. Turgeson, A., Harris, B. Elucidation of the mechanism of long-chain fatty acid recognition in *V. cholerae*: an in silico study. American Institute of Chemical Engineers Annual Meeting 2020 November 15-20; San Francisco, CA (abstract accepted for conference paper).

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

1. Continued collaboration with Dr. David Giles, UTC Department of Biology, Geology, and Environmental Science and Dr. Jin Wang, UTC Department of Mathematics.
2. New collaboration with Dr. Shawn Campagna, UTK Biological and Small Molecule Mass Spectrometry Core and Biomembranes Community of Scholars.
3. New collaboration with Dr. Jeremy Smith, UTK/ORNL Center for Molecular Biophysics.
4. New collaboration with Dr. Jerome Baudry, UAH Biological Sciences Department.

EXTERNAL FUNDING

Proposal Submissions

1. NSF CAREER, CAREER: Developing a mechanistic model for unsaturated fatty acid recognition in Gram-negative bacteria ($519,000, 2/1/21-1/31/25)

Contracts/Awards Received

1. NIH R15 Award #1R15GM131315-01A1, Experimentally Guided Modeling and Simulation for Cholera Dynamics ($340,000, 9/1/19-8/31/22)

Sponsored Program Capacity Building Activities

1. Prepared NSF CAREER proposal draft for external reviewers secured by UTC's Office of Research and Sponsored Programs.
2. Virtual meeting with Dr. David Rockcliffe, PO for NSF BIO MCB Systems and Synthetic Biology cluster.

WHAT'S NEXT FOR THIS RESEARCH?

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

My long-term career goal is the establishment of a world-class interdisciplinary systems and synthetic biology research group for advancing applications in biotechnology while providing undergraduate and graduate STEM students with valuable training and hands-on research experiences. My group's long-term goal in this research is to understand how the capacity for UFA uptake and utilization in bacteria is intrinsically linked with fitness and resistance phenotypes. I have demonstrated the dependence of fitness and resistance phenotypes on both UFA availability and environmental conditions in *Vibrio cholerae* (or *Vc*). I have shown that *Vc* possesses multiple fatty acid transporter homologs whose structural dissimilarities may explain its ability to uptake a more diverse range of UFAs compared to *E. coli*. These results have positioned us to now identify the common pathways and molecular mechanisms involved in UFA recognition in Gram-negative bacteria, which is the focus of my NSF CAREER application.

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

I intend to pursue the research outlined above in collaboration with UTK's Biological and Small Molecule Mass Spectrometry Core and Biomembranes Community of Scholars, as well as ORNL's Center for Molecular Biophysics.

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 two most likely barriers to these future goals are (1) lack of university/college/departmental support for state-of-the-art experimental facilities, and (2) insufficient recruitment of and support for exceptionally talented students in the M.S. engineering and Ph.D. computational engineering programs.

FINANCIAL ACCOUNTING

$11,235.29 from the award remains to be spent. Due to the COVID-19 pandemic, $8,200 was approved for carryover into the new fiscal year. This includes $3,200 for student pay and $5,000 for conference travel. This leaves approximately $3,035 in unspent funds. This can be attributed to unfinished experimental trials halted by closure of facilities during the pandemic, which resulted in forecasted materials and supplies not being purchased for use.

Fiscal Year 2020 Final Project Report

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

Dr. Jennifer Hogg, Lead PI

Co-PI(s): Shellie Acocello, Yu Liang, Dalei Wu, Gary Wilkerson

Project Title: "The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation"

Date Submitted: 08/03/2020

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

Non-Technical Summary:

As many as 23% of individuals who undergo surgical reconstruction of the anterior cruciate ligament will re-injure the same knee or the opposite knee within two years after return to normal activities. Current practice does not emphasize the importance of disrupted brain processes that are crucial for integration of sensory inputs and generation of effective muscle activations for maintenance of dynamic joint stability. Augmented reality may provide visual challenges and user feedback that promote brain adaptations needed for restoration of optimal function after musculoskeletal injury, or enhancement of performance capabilities within other populations. For example, recent evidence has documented that concussion elevates risk for subsequent sport-related musculoskeletal injury in the lower extremity approximately two-fold.

A virtual reality system was developed, which has provided data used to assess hypothesized relationships among factors believed to influence maintenance of dynamic stability of the knee joint, as well as that of other joints influencing lower extremity alignment. A graduate research project involving Ashley Williams, Samantha Kendall, and Colton Jenkins, entitled "OPTIMAL-Based Virtual Reality Feedback to Reduce Dual-Task Balance Cost," was presented in the 2020 Virtual Meeting of the American Society of Biomechanics and is currently being prepared for submission as a full manuscript. Another graduate research project utilized one component of the same system (the virtual reality environment developed by Griffin Miller, computer science undergraduate), which involved Meredith Davis, Justin Ramos, and Abigail Rucker. A research manuscript derived from their data, entitled "Wellness Survey Responses and Smartphone App Response Efficiency Associate with Remote History of Sport-Related Concussion," is currently under peer review by the journal Perceptual and Motor Skills. Final data reduction is ongoing, and at least one other manuscript is anticipated. These scholarly outputs clearly demonstrate the potential benefits of new technological applications developed by the SimCenter to the advancement of sport-related injury prevention and rehabilitation.

PROJECT TITLE: The Use of Augmented Reality-Delivered Feedback to Train Neurocognitive and Neuromuscular Deficits: A Preliminary Investigation
Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
Dual-task tests of combined cognitive and motor demands are believed to provide data that reflect the efficiency and accuracy of brain integration of visual, cognitive, proprioceptive, and motor processes. Virtual reality (VR) and augmented reality (AR) applications can provide complex visual stimuli that are expected to reveal meaningful insights about functional impairment and potential improvement of cognitive-motor function. • Potential participants screened to identify those with suboptimal ability to maintain low-risk knee alignment during a single-leg squatting movement. • Determination of the immediate and delayed impact of VR-delivered feedback on 3-dimensional biomechanics during a single-leg squat under both single- and dual-task conditions. • Separate project utilized VR-delivered cognitive test to identify any performance differences between individuals who self-reported history of sport-related concussion from those who denied such a history.	• "OPTIMAL-Based Virtual Reality Feedback to Reduce Dual-Task Balance Cost" presented in the 2020 Virtual Meeting of the American Society of Biomechanics and is currently being prepared for submission as a full manuscript. • Machine learning analysis of full dataset currently being completed for inclusion in another manuscript that will report results closely aligned with the primary project aim ("Effect of OPTIMAL motor learning theory application on single- and dual-task biomechanics of the lower extremity"). • "Wellness Survey Responses and Smartphone App Response Efficiency Associate with Remote History of Sport-Related Concussion" currently under peer review for possible publication in Perceptual and Motor Skills. • OPTIMAL theory influences on kinematic and kinetic changes is in analysis and will be an outcome.
RESULTS	**OTHER INFO**
	Budget and Schedule Total Budget: $90,538.00 Actual Used: $90,538.00 Balance: $ 0.00 Total period of performance is 12 months Task 1: Months 1-3—IRB approval, VR development Task 2: Months 4-6 –Participant recruitment, data collection

	Task 3: Months 6-9—Data collection, data screening Task 3: Months 10-12—Data reduction, analysis, manuscript preparation **Deliverables** • VR system development • Final project report. • Professional conference presentation • Publications (1 currently under review; 2 additional manuscripts currently under development for submission) **Organization Information** N/A

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop AR system to assess the application of the OPTIMAL theory of motor learning on single and dual-task biomechanics.	VR system developed and deployed for documentation of improvement in the ability to maintain low-risk knee alignment during dual-task dynamic activity.
Develop innovative methods to assess functional deficiencies that result from lower extremity musculoskeletal injury or mild traumatic brain injury.	VR Flanker Test with pupil tracking developed and deployed for assessment of long-term effects of sport-related concussion on cognitive-oculomotor function.
Teach graduate students in Athletic Training in methods for acquisition and analysis of data from a 3-dimensional motion tracking system.	Students acquired sufficient competency to independently perform similar data collection and analysis activities.
Teach graduate students in Athletic Training how to prepare research results for professional conference presentation and publication.	Students acquired sufficient competency to serve as co-authors for conference presentations and peer-reviewed journal manuscript submissions.

Challenges & Strategies Used to Address / Overcome:

Construction in MAPP building was an early challenge that greatly impeded scheduling of data collection sessions. Meetings with the construction personnel were essential to know when electrical power would not be available and to stay aware of any other constraints that would affect data collection efficiency. Scheduling data collection sessions was also limited by the

availability of health profession graduate students who had competing clinical education assignments that severely restricted options.

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

Although we initially planned to develop an AR environment, the latency was too great to allow for fluid movement, thus we reverted to a VR environment. Developing an AR system in the future will require consulting with outside sources and purchasing more equipment. The pupil tracking system integrated with the VR headset repeatedly malfunctioned, which necessitated shipping to Germany on two occasions for correction of problems. The technology has advanced over the past couple of years, which now provides other hardware and software options for quantification of rapid eye movements under dynamic conditions. Additionally, the test we designed for quantification of eye responses to visual stimuli did not provide measurements with good test-retest reliability. The visual target for response registration may have been too small, which might have prolonged the elapsed time between appearance of the visual stimulus and eye movement to the spatial coordinate required or registration of the response. Future measurements of eye responses will define response time on the basis of a pre-specified amount of pupil displacement in the correct direction.

IMPACT & OUTCOMES

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

The project provided pilot data for an upcoming R15 REAP Grant application, which will include a co-investigator who provided highly specialized consultation that was funded by the CEACSE grant (Jed Diekfuss, PhD). Graduate students in Athletic Training had the opportunity to discover the clinical relevance of technological applications for assessment of functional capabilities, whereas those in Computer Science had the opportunity to experience real-world application of a data acquisition system that they helped to create. Each faculty member engaged in the project gained a deeper understanding of both the challenges and opportunities that accompany research pertaining to neurocognitive and neuromuscular interrelationships. The innovative nature of the project will undoubtedly advance conceptualization of future related work, which appears to offer potential for substantial impact on clinical management of sport-related injuries.

Students Impacted

Graduate students in Athletic Training (May 2020 graduation with MSAT degree); 2 research project groups: 1) Ashley Williams, Samantha Kendall, and Colton Jenkins; 2)Meredith Davis, Justin Ramos, and Abigail Rucker. 3) Computer Science & Engineering students: Griffin Miller, Zoe Zimmerman, Nicholas Milburn

Community and Broader Impacts

The societal impact of the project could prove to be substantial. The strongest predictor of any type of sport-related injury is a prior injury, which is likely due to the inadequacy of the prevailing clinical approach to injury prevention and treatment. Emerging evidence, including that derived

from our own research, strongly supports the importance of efficiently integrated cognitive-motor processes in the brain for generation of effective responses to rapidly changing environmental circumstances. Because repetitive sports injuries often lead to dysfunction and progressive disability, the nature of the project offers the potential for reduction of neurological degeneration and osteoarthritis.

Scholarly Products

Publications:

1. Hogg, J., Wellness Survey Responses and Smartphone App Response Efficiency Associate with Remote History of Sport-Related Concussion, Perceptual and Motor Skills (under review)

External Conferences:

1. Hogg, J., OPTIMAL-Based Virtual Reality Feedback to Reduce Dual-Task Balance Cost, 2020 Virtual Meeting of the American Society of Biomechanics (will be refereed in the Journal of Biomechanics)

Presentations at UTC:

1. Both graduate student research projects were scheduled for presentation at the Research Dialogues Conference that was cancelled.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

Both the project PI (Jennifer Hogg) and one of the collaborating UTC researchers (Gary Wilkerson) recently served as co-authors with prominent researchers in the specific field of cognitive-motor assessment and rehabilitation for reduction of risk for future knee injury. Two of these key clinical researchers (Jed Diekfuss, PhD and Greg Myer, PhD) recently accepted new positions in close proximity to UTC (Emory University). Opportunity clearly exists for further collaboration between these parties, in addition to UTC Athletic Training collaborations with those in Computer Engineering. Both development of new technology for data acquisition and utilization of machine learning for data analysis appear to offer numerous opportunities.

EXTERNAL FUNDING

Proposal Submissions

1. An R15 AREA NIH proposal entitled “A New Paradigm for Sport Injury Prevention and Reduction of Risk for Disability” that was submitted in February 2020 included the CEACSE project PI (Jennifer Hogg) as a co-researcher and one of the participating researchers as PI (Gary Wilkerson). A review summary statement was recently received that included very good reviewer scores, which suggests that the potential for funding of a revised proposal is

promising. A revision is currently being prepared for submission in October, which includes a Computer Engineering faculty member as a co-investigator (Mina Sartipi, PhD).

Contracts/Awards Received

1. None

Sponsored Program Capacity Building Activities

1. None

WHAT'S NEXT FOR THIS RESEARCH?

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

An R15 REAP NIH proposal is under development for submission to the National Institute for Arthritis, Musculoskeletal, and Skin Diseases in February 2021 (PI: Jennifer Hogg).

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

Refinement of the VR system developed for the project will be continued (Yu Liang, PhD and Dalei Wu, PhD) for future use in continuing research relating to motor learning theory for optimization of knee function. Collaboration will be continued with closely related research in the area of sport-related concussion assessment and reduction of risk for subsequent musculoskeletal injury (Gary Wilkerson, EdD). Incorporation of machine learning in quantification of risk for sport-related injury will promote continued collaboration with Computer Engineering (Mina Sartipi, PhD). These interrelated activities may present good opportunity for development of telehealth applications that will facilitate home-based assessments and therapeutic exercise interventions.

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

Neither the Athletic Training profession or the broader field of Sports Medicine have made much progress to date in transitioning from reductionist thinking to a complex systems approach to research and clinical practice. Great opportunity clearly exists to assume the role of a leading institution in the inevitable progression toward increased reliance on technology for guidance of clinical practice.

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

Availability of release time from teaching responsibilities is necessary for an optimal rate of continued progress, along with funding for graduate research assistants. Another barrier to realization of opportunities that currently exist is the exceedingly slow process of obtaining the funding required to develop and refine innovative technology applications.

FINANCIAL ACCOUNTING

We zeroed our budget and accomplished our aims. The only budget glitch we had was that some monies allocated for student workers were accidentally billed to another grant. It was caught eventually. Would likely have been prevented through more oversight from the PI.

Fiscal Year 2020 Final Project Report

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

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

Co-PI(s): Dr. Jejal Reddy Bathi and Dr. Mark Schorr

Other Personnel: Mr. Richard Blanton - Graduate Student (Research Assistant), Mr. Caleb Mathias - Undergraduate Student (Research Assistant), Mr. Shuvashish Roy - Graduate Student (Research Assistant), and Mr. Syed Tareq - Graduate Student (Research Assistant).

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

Date Submitted: 08/16/2020

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

Non-Technical Summary:

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

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

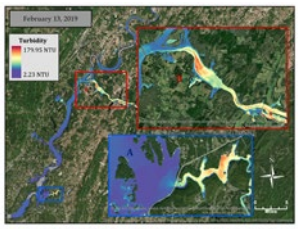
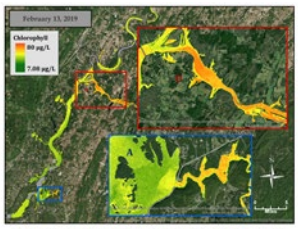
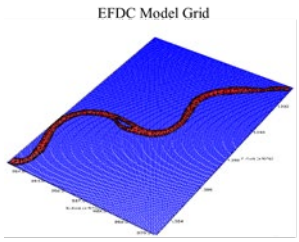
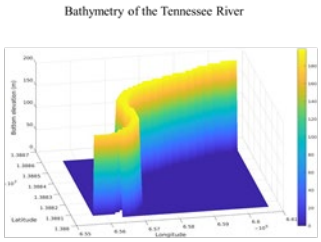
Environmental Remote Sensing Laboratory (GERSLab) at UTC by providing new water quality measuring equipment and resources.

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

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

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

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

TECHNICAL APPROACH	OUTCOMES
Integration of satellite observations with numerical models to estimate hydro-dynamically computed surface water quality parameters in the watersheds of southeast Tennessee. List of tasks: (1) Geospatial/satellite data acquisition and processing, (2) In situ water quality data acquisition, (3) Remote sensing-based water quality estimation, (4) Numerical model development and application, (5) Water quality parameters estimation using Numerical model coupled with satellite observations, and (6) Report generation and publications.	The outcomes of this project include: (1) several conference presentations, a book chapter, and research data and results for preparing several journal articles and seeking external funding opportunities; (2) potential proof of concept of remote sensing-integrated water quality modeling capability; and (3) support and contribution to advance SimCenter's mission in the environment research thrust by developing new innovative research at UTC on surface water quality modeling and simulation.
RESULTS	**OTHER INFO**
Developed satellite observed water quality estimation models for the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek.  Estimation of Turbidity using Landsat 8 OLI image acquired on February 13, 2019  Estimation of Chlorophyll concentration using Landsat 8 OLI image acquired on February 13, 2019 *Developed EFDC 3D model for the Tennessee River flows (flow depth, flow velocity, and flow quantity)*  EFDC Model Grid  Bathymetry of the Tennessee River	**Budget and Schedule** Total Budget: $96,488.00 Actual Used: $78,620.94 Balance: $17,867.06 Approved carryover for 2021 fiscal year (Due to COVID-109): $ 14,200.00 Total period of performance is 12 months. Task 1: Months 1-8, Task 2: Months 1-8 Task 3: Months 1-9, Task 4: Months 1-8 Task 5*: Months 8-11, Task 6: Months 3-12 * Remain Incomplete due to COVID-19. **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication, and external and internal conference presentation **Organization Information** Dept. 2653, 615 McCallie Avenue Chattanooga, TN 37403, Ph: 423-425-4404 Email: azad-hossain@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

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

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

<table>
<tr><th>List of Objectives / Aims / Major Milestones Proposed</th><th>Cumulative Outcomes / Accomplishments</th></tr>
<tr><td>Task 1. Geospatial/satellite data acquisition and processing</td><td>Collection and processing of different multispectral satellite imagery. The acquired and processed satellite imagery are as follows:
One scene of Landsat 8 OLI multispectral image acquired over part of the Tennessee River on August 15, 2019.
Several scenes of high-resolution multispectral images acquired by the Plant Dove satellites (PlanetScope) over part of the Tennessee River on August 14-16, 2019 and October 22, 2019.
Once scene of Sentinel-2 multispectral imagery acquired over the Tennessee River on October 22, 2019.</td></tr>
<tr><td>Task 2. In situ water quality data acquisition</td><td>Collection of in situ water quality measurements in selected parts of the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek.
Acquired near-real time (with satellite image acquisition) in situ water quality data (Temperature, pH, Turbidity, Chlorophyll, Dissolved Oxygen, and Conductivity) for about 30 stations in and around South Chickamauga Creek on August 15, 2019; and for about 50 stations in the Tennessee River near downtown and around South Chickamauga Creek on October 22, 2019.</td></tr>
<tr><td>Task 3. Remote sensing-based water quality estimation</td><td>Development of different satellite observed water quality estimation models for the Tennessee River, Chickamauga Lake, and Lower South Chickamauga Creek.
A series of numerical models have been developed to estimate turbidity, chlorophyll, conductivity, pH, and Dissolved Oxygen (DO) using Landsat 8 OLI imagery (Task 2) and concurrent in situ water quality measurements (Task 1). The following table shows the selected regression equations and correlation coefficients for each water quality parameter.
<table><tr><th>Parameter</th><th>Band(s)</th><th>Regression Type</th><th>Equation</th><th>R^2</th></tr><tr><td>Turbidity</td><td>4</td><td>Nonlinear Exponential</td><td>$Turbidity = 1.769 * e^{0.284 * \rho_{red}}$</td><td>0.95</td></tr><tr><td>Chlorophyll</td><td>1,2,3</td><td>Linear Multi-Regression</td><td>$Chlorophyll = 10.37 + 29.55 * \rho_{coastal} - 39.41 * \rho_{blue} + 12.90 * \rho_{green}$</td><td>0.66</td></tr><tr><td>DO</td><td>5</td><td>Nonlinear Power</td><td>$DO = 11.405 * \rho_{NIR}^{-0.11}$</td><td>0.72</td></tr><tr><td>Conductivity</td><td>5</td><td>Nonlinear Exponential</td><td>$Conductivity = 181.64 * e^{-0.069 * \rho_{NIR}}$</td><td>0.45</td></tr><tr><td>pH</td><td>2,3,4</td><td>Linear Multi-Regression</td><td>$pH = 7.716 - 0.165 * \rho_{blue} + 0.145 * \rho_{green} - 0.076 * \rho_{red}$</td><td>0.42</td></tr></table>
Several numerical models have also been developed to estimate selected water quality parameters using Sentinel-2 and Planetscope imagery (Task 2) and concurrent in situ water quality measurements (Task 1).</td></tr>
<tr><td>Task 4. Numerical model development and Application</td><td>As a part of this task, a detailed hydrological watershed model using the Hydrological Simulation Program--Fortran (HSPF) model for south Chickamauga Creek watershed was developed such that the watershed hydrology and water quality can be simulated on continuous basis. However, in order to simulate lateral discharges into the Tennessee River, with synchronized efforts with another CEACSE project, a detailed HSPF</td></tr>
</table>

	watershed model was also set-up for North Chickamauga Creek. Both of these watersheds are located below the Chickamauga Reservoir. As part of this task, in collaboration with research funded by the United States Geological Survey through the Tennessee Water Resources Research Institute, a three-dimensional hydrodynamic model was developed and calibrated for a portion of the Tennessee River such that fate and transport of water quality parameters in the river can be quantified. The model developed using Environmental Fluid Dynamic Code (EFDC). The developed model was calibrated for hydraulics by comparing monitored flows and flow depth in the river. However, the model is yet be calibrated for water quality parameters.
Task 5. Water quality parameters estimation using Numerical model coupled with satellite observations	Due to COVID-19 Pandemic this task remained incomplete. The obtained no-cost extension and approved carry-over fund would provide with the opportunity to complete this task.
Task 6. Report generation and publications	Three quarterly progress reports were prepared and submitted to report the progress of the project. The project produced one book chapter, 5 external conference presentations, and 2 internal (UTC) research presentations. One manuscript is in preparation for peer reviewed publications. Several other manuscripts will also be prepared for peer reviewed publications.

Challenges & Strategies Used to Address / Overcome:

Challenges	**Strategies Used to Address / Overcome**
1. Sometimes it was very difficult to obtain a cloud free satellite imagery. It becomes even more challenging due to large temporal frequency of Landsat satellite (16 days) missions.	Used other optical satellites of similar spectral characteristics (such as PlanetScope and Sentinel-2) in addition to Landsat 8 satellite.
2. Frequent cloud coverage over the study site kept it challenging to acquire more in situ water quality measurements along with near-real-time satellite imagery, especially after storm events.	Used other optical satellites of similar spectral characteristics (such as PlanetScope and Sentinel-2) in addition to Landsat 8 satellite.
3. The purchase of the new water quality measuring sonde was delayed as the paper works for procurement process took more time since the vendor was not registered with UTC.	Necessary efforts had been made to expedite the procurement process of the sonde. The sonde was finally received early March 2020.
4. The watershed and hydrodynamic modeling have been delayed by the Co- PI's team.	Necessary efforts had been made to expedite the modeling efforts.

5. We had to postpone several field trips (to measure Nitrate, Chloride, and Ammonium) and laboratory works due to current COVID-19 situation. These activities will be needed to resume after summer to accomplish several proposed tasks of the project. These tasks are heavily dependent on the students/research assistants' assistance.	We requested to obtain no-cost extension of the project and carryover some funds to support students' work and travels in the next fiscal year. We have received the approval of our request.
6. The PI was supposed to attend the 2020 GSA Joint Section Meeting in Reston, VA in March to present some preliminary results of the project, but it was canceled due to COVID-19 situation.	We have plan to attend GSA Section Meeting 2021 in Auburn, AL on April 1-2, 2021.
7. The PI and the students were supposed to attend the UTC Research Dialogue 2020 in April to present some preliminary results of the project, but it was canceled due to COVID-19 situation.	We submitted one poster on UTC's virtual scholar's platform and planned to present during future Research Dialogue events.

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

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

IMPACT & OUTCOMES

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

Impact on the Career of the PI:

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

the research data and generate publishable results and thereby increased my capacity to successfully compete for tenure.

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

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

Impact on the Career of the Cp-PIs:

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

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

Students Impacted

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

Caleb Mathias: Mr. Mathias is a recently graduated undergraduate student in Geology. He joined GERS Laboratory at UTC at the beginning of fall 2019 as a term research assistant for this project. This project provides him with the opportunity to conduct water quality remote sensing research and how it can be integrated with numerical hydrodynamic and watershed models. He is gaining valuable post baccalaureate research experience through this project. This unique research experience helps him to get ready for pursuing higher education and/or starting professional or research career in this area. Mr. Mathias has been admitted in the

graduate program at the University of British Columbia (UBC) in Canada with full research assistantship. He will join UBC in fall 2021.

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

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

Community and Broader Impacts

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

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

Scholarly Products

Publications:

1. Hossain, A., Blanton, R., and Mathias, C., Remote Sensing of Surface Water Quality in Southeast Tennessee. The manuscript is under preparation and to be submitted to Remote Sensing of the Environment.

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

External Conferences:

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

2. Hossain, A., Blanton, R., and Mathias, C., 2019, Surface Water Quality Monitoring Using Remote Sensing Technology in Chattanooga. SWPBA 46th Annual Meeting in Chattanooga, TN October 14th to 17th, 2019.
3. Hossain, A., Blanton, R., and Mathias, C., 2019, Quantitative Remote Sensing of Surface Water Quality in Southeast Tennessee. AGU Fall Meeting, 9-13 December 2019, San Francisco, CA.
4. Roy., S., Atolagbe., B., Ghasemi., A., Bathi., J. R. “A MATLAB-based Grid Generation Tool for Hydrodynamic Modeling” ASCE Environmental and Water Resource Institute (EWRI) Conference, Henderson, NV, May 17 – 21, 2020.
5. Hossain, A., Blanton, R., and Mathias, C., 2019, 2020, Quantitative Remote Sensing of Surface Water Quality in Southeast Tennessee Utilizing Planet Dove Imagery, 69th Annual Southeastern / 55th Annual Northeastern Section Meeting – 2020, 20-22 March 2020, Reston, Virginia (Abstract accepted). Conference canceled due to COVID-19 situation.

Presentations at UTC:

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

Inventions or Other Intellectual Property

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

Research Outreach & Collaboration

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

This study can be considered as a follow-up and complementary to UTC's "Urban Streams Project" (1998-2000) as it is monitoring selected streams in the Chattanooga area (Tennessee-Georgia). The obtained research results provide valuable information on the health

of the City's stream ecosystems. Such information can be utilized by the City of Chattanooga, the Tennessee Department of Environment and Conservation (TDEC), the Tennessee Wildlife Resources Agency (TWRA), the Tennessee Aquarium Conservation Institute, and the Tennessee Valley Authority. Currently we have started a research project with TWRA. Recently we also submitted a research proposal to City of Chattanooga related to this project. We had research collaboration meetings with TDEC to synchronize their field data collection program with satellite image acquisition.

EXTERNAL FUNDING

Proposal Submissions

- Integration of Remote Sensing Technology with Hydrodynamic Models for Surface Water Quality Monitoring in Southeast Tennessee, Agency: USGS through Tennessee Water Resources Research Center (TNWRRC). Duration: March 1, 2020 - February 28, 2021. Total amount: $24,976 (Federal) and $50,390 (Non-federal). Role: Principal Investigator. Not funded.

- Urban Streams Restoration Project: Measuring the Efficacy of Habitat Mitigation/Restoration Efforts on Chattanooga Area Streams: Citico Creek, Friar Branch, and Mountain Creek. Agency: City of Chattanooga. Duration: 01/01 /2020 - 08/ 31/ 2022. Amount: $275,907. Role: Co-Principal Investigator (Principal Investigator: Mark Schorr). Pending.

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

Contracts/Awards Received

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

Sponsored Program Capacity Building Activities

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

WHAT'S NEXT FOR THIS RESEARCH?

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

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

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

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

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

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

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

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

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

FINANCIAL ACCOUNTING

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

Fiscal Year 2020 Final Project Report

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

Dr. Hamdy Ibrahim, Lead PI

Co-PI(s): Mohammad Mahtabi

Project Title: "CORROSION MODELING OF MAGNESIUM-BASED FIXATION HARDWARE FOR MANDIBULAR RECONSTRUCTION SURGERIES"

Date Submitted: 08/10/2020

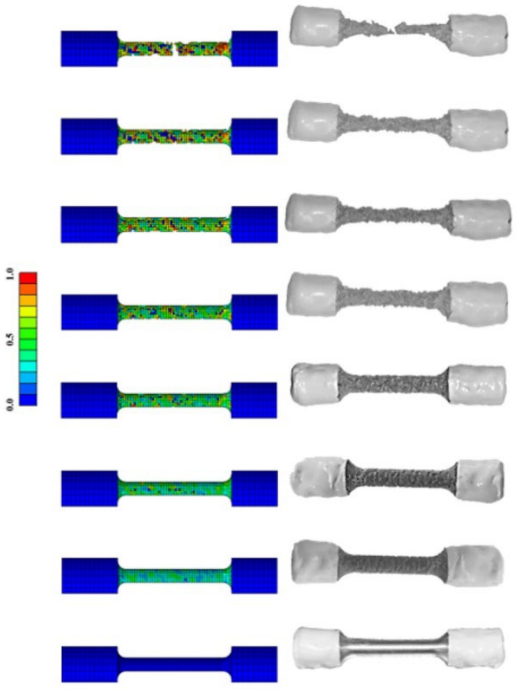
Award Start – End Date: July 1, 2019 – June 30, 2020

Non-Technical Summary:

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

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

Technology Area of Interest: Health & Biology Systems

TECHNICAL APPROACH	OUTCOMES
• Developing the subroutine (code) that can simulate the corrosion behavior of Mg alloys using the continuum damage mechanics theory. • Calibrating and validating the subroutine parameters using in-vitro immersion test results.	A code was developed based on the continuum damage mechanics theory for the pitting corrosion, compressive stress corrosion, and tension stress corrosion to assess the overall damage as corrosion proceeds. model was calibrated by conducting a series of tests in conditions simulating the body environment. The results of this work resulted in the submission of 2 journal papers, 1 conference presentation and 2 NSF proposals.
RESULTS	**OTHER INFO**
	**Budget and Schedule** Total Budget: $99,905.99 Actual Used: $81,666.91 Balance: $ 13,239.08 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-6 Task 3: Months 6-12 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication • External and internal conference presentation **Organization Information** *Address, Phone, and Email*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

Challenges & Strategies Used to Address / Overcome:

The main challenge we faced was the lockdown due to the COVID19 situation which resulted in a delay with the corrosion testing work. We managed to perform most of the needed tests especially the immersion test work. However, we conducted some of the needed tests during Summer and will continue the rest of the testing during the Fall semester.

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

N/A

IMPACT & OUTCOMES

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

The PIs gained a fundamental understanding of corrosion modeling of magnesium alloys as a new class of regenerative skeletal fixation devices using continuum damage mechanics. The project also enhanced the available infrastructure for the PIs and other researchers at the UTC to conduct future research on the corrosion of metals and other activity in the area of biodegradable materials. Finally, the pilot data of this project and the provided support helped the PIs to prepare and submit two NSF proposal and to submit 2 journal papers.

Students Impacted

- Moataz Abdalla, Masters student: He was completely funded and led the students' effort in this project for one year. He is expected to graduate Spring 2021.
- Austin Sims, Masters student: He was partially funded in this project. He is expected to graduate Fall 2020.
- Alexander Joplin, Undergraduate student: He was partially funded in this project during Spring and Summer 2020.
- Clay Jones, Undergraduate student: He was partially funded in this project during Spring 2020.

Community and Broader Impacts

The broader impacts of the conducted work on the advancement of a medical device made of biodegradable metals are substantial. Current modalities of treating patients with bone trauma rely on the use of permanent and stiff bone fixation devices (e.g. Ti-6Al-4V and 316L stainless) that carry substantial risks of inflammation, infection, subsequent bone fracture, and bone resorption. This usually requires physicians to perform a second implant removal surgery after bone healing which increases the suffering of patients and the total operation cost. The success in developing nonpermanent bone fixation devices that can address the problems associated with the currently-in-use permanent ones will result in a clinical breakthrough. Two graduate students and two undergraduate students were involved in this project. They learned about the technical aspects of the project in addition to giving presentations about their work.

Scholarly Products

Publications:

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

External Conferences:

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

Presentations at UTC:

N/A

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

1. **Ibrahim, H.**, "Treating Bone Trauma Using ResorbFix", I-Corps Teams, submitted to the National Science Foundation (NSF), 2020. Requested amount: $50,000.
2. **Ibrahim, H.,** Mahtabi, M., Danquah, M., Elliot, T., Palchoudhury, S., Elliot, L. & Panagiotou, E. "Acquisition of a customized metal additive manufacturing system for multidisciplinary research activities", Major Research Instrumentation Program: (MRI), submitted to the National Science Foundation (NSF), 2020. Requested amount: $261,500.

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

N/A

WHAT'S NEXT FOR THIS RESEARCH?

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

I will continue m research on the biodegradable metals for the intended biomedical applications with more focus on expanding the collaboration to follow-on studies looking at an in vitro cytotoxicity testing and in vivo animal studies.

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

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

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

N/A

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

N/A

FINANCIAL ACCOUNTING

Just Due to the COVID19 situation, the remaining balance was accepted for a carry-over during the 2020/2021 fiscal year to support students and/or travel to continue the remaining experimental work when we are able again.

Fiscal Year 2020 Final Project Report

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

Dr. Farah Kandah, Lead PI

Co-PI(s): Mina Sartipi

Project Title: “Decentralized and scalable trust management approach via blockchain for connected vehicles in smart cities.”

Date Submitted: 07/31/2020

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

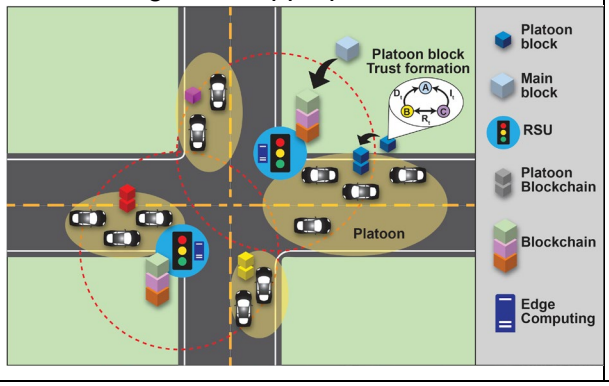
Non-Technical Summary:

Our project aims to support smart cities dynamic setups such as connected vehicles, through the creating a trustworthy relationships that are tamper proof in order to provide a secure and trustworthy environment to ensure that real-time decisions are made with confidence that the data being shared between the entities are legitimate and originated by trustworthy entities in the system.

The work conducted throughout this research project offered significant contributions to the field of trust management and blockchain applications. A novel trust management algorithm was developed that was better able to mitigate threats than previous trust implementations. Blockchain applications were researched and the foundational setup to a laboratory for testing and implementation purposes to evaluate the applicability of Blockchain in the IoT environment.

The advancements made throughout this project are critical to the future successes of UTC’s SimCenter. Not only were significant academic achievements made in the areas of trust management and blockchain, but the research and development advancements made with the Internet of Things laboratory will aid in future efforts made by the SimCenter and the researchers within it. As continued discovery and setup steps are taken this IoT lab will be critical to later works as it will allow for accurate representation and simulation of IoT devices within a smart infrastructure.

PROJECT TITLE: Decentralized and Scalable Trust Management Approach via Blockchain for Connected Vehicles in Smart Cities
Technology Area of Interest: Cybersecurity and Cyber-physical systems

TECHNICAL APPROACH	OUTCOMES
• Develop a dynamic trust management approach that is applicable to smart cities setups • Investigate Blockchain setups to develop a IoT applicable Blockchain testbed	- F. Kandah, B. Huber, A. Altarawneh, S. Medury and A. Skjellum, "BLAST: Blockchain-based Trust Management in Smart Cities and Connected Vehicles Setup," 2019 IEEE High Performance Extreme Computing Conference (HPEC), Waltham, MA, USA, 2019, pp. 1-7, doi: 10.1109/HPEC.2019.8916229. - F. Kandah, A. Altarawneh, B. Huber, A. Skjellum, and S. Medury, "A Human-Understandable, Behavior-based Trust Management Approach for IoT/CPS at Scale," Int. J. of International Society for Computers and Their Applications (ISCA), In Press (2020) - J. Coleman, F. Kandah, and B. Huber, "Behavioral Model Anomaly Detection in Automatic Identification Systems (AIS)," In 2020 IEEE 9th Annual Computing and Communication Workshop and Conference (CCWC) - Accepted 2020. - In progress: Brennan Huber is completing his thesis based on work being done during this project.
RESULTS	**OTHER INFO**
Include a figure as appropriate. 	Fill in your info below. **Budget and Schedule** Total Budget: $100,000.00 Actual Used: $62,019.88 Balance: $ 37,980.12 Total period of performance is 12 months. Task 1: Trust management -- Months 1-5 Task 2: Secure and Distributed Trust Database -- Months 3-9

	Task 3: Edge Computing -- Months 1-9 Task 4: Evaluation -- Months 6 - 12 **Deliverables** • Quarterly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publication **Organization Information** University of Tennessee Chattanooga Computer Science and Engineering 615 McCallie Ave., Chattanooga, TN 37403 Farah-kandah@utc.edu 423-425-4395

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Prototype the trust factor and modification model to evaluate and ensure that the vehicle's trust factor accurately reflects the truthfulness of its messages.	Created a new trust management algorithm to incorporate four variables that will be used together to combat unique threat models.
Analyze and evaluate the hash matrix generation, aiming to reduce any additional overhead on the vehicle. Further assessment will be done to determine the optimal size of the matrix and how often there is a need to re-create a matrix/chain to avoid any masquerading attacks in the network.	IoT lab foundation setup began including numerous Raspberry Pis as well as Raspberry Pi remote controlled cars that were developed and tested to be used for future projects involving V2V communication.
Prototype the blockchain instance and evaluate the optimal platoon hash size that the vehicle is capable of calculating while taking the block time into consideration.	Developed a behavioral model that can assist the trust management in a dynamic scenario
Prototype the blockchain instance and evaluate the optimal number of platoon blockchains to pack into the main block before the mining process begins.	Developed a behavioral-model based trust management that is used to describe how vehicles in a specific area are expected to drive. Integrated the behavior of vehicles in the evaluation of a vehicle's trustworthiness.
Utilize edge computing to address the transmission delay requirement for time-sensitive applications.	By merging edge computing and caching units, we introduced multivariable optimization for quality of service that analyses wireless network performance. For data analysis applications, we executed machine learning at the edge to alleviate the transmission delay. For applications that required access to popular content, caching at local access points was used.
Run various evaluations experiments for the time vs. storage complexity, as well as hardware testing to determine the demand on the resources.	Investigated the development of blockchain-based IoT systems to aid in the creation of our own IoT and blockchain laboratory.

Challenges & Strategies Used to Address / Overcome:

The Covid-19 restrictions delayed the progress of the project in the last quarter where there was an inability to access the laboratory and we were not able to build the testbed and be able to evaluate the applicability of Blockchain in IoT setups on a larger scale. As we are getting back on campus, we are planning to get the testbed built and start the testing and evaluation as soon as we finish the build. Materials were acquired but we were not able to build it yet.

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

Due to the system dynamicity, the velocity of the vehicles as well as the time taken to elect a miner had significant impacts to the effectiveness of blockchain technology. As the velocity range of vehicles increased, the number of blocks that a platoon of vehicles was able to successfully complete drastically decreased due to the limitation in the DSRC transmission range. This also explains the miner election timing because as the time to elect miner increases the distance between the vehicles becomes greater and greater thus the number of blocks would also decrease.

IMPACT & OUTCOMES

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

This proposal added to the PIs experience in the field of Smart cities and connected vehicles.

The PIs were able to extend their research into the field of IoT and apply for external funding opportunities related to this research. During the period of performance and in support for future research endavious, the PIs initiated a number of collaborations with researchers from the Electrical Engineering department at UTC, and Computer Science Departments at TTU, and MTSU.

Students Impacted

Brennan Huber, M. Sc Computer Science: Cyber security. During the period of performance, Mr. Huber acquired a good amount of experience into coding and developing and evaluating the system.

Amani Altarawneh, PhD Computational Science: Computer Science. Ms. Altarawneh acquired a great experience related to designing Blockchain approaches that is applicable to IoT systems setup.

Sai Madury, PhD Computational Science: Computer Science. Mr. Madury acquired a great experience in programming and dealing with OpenStack clustering to develop and simulate a Blockchain based communication system to evaluate the applicability of Blockchian in dynamic system setups.

Jacob Coleman, M.Sc. Computer Science. Mr. Coleman acquired a great experience in machine learning and how it related to different applications in smart cities setups including trust management in IoT systems (specifically Ocean of Things).

Jonathan Hunter, M.Sc Computer Science. Mr. Hunter investigated the applicability of Blockchain in IoT systems which provided him with a great understanding of how Blockchain can assist in providing a tamper proof, global view of the data shared among the system's entities. Also, he acquired good experience in coding and developing using Raspberry Pis.

Sree M.Sc. Computer Science. Ms. Sree implemented a computer vision (CV) algorithm on edge and was introduced to different CV algorithms.

Community and Broader Impacts

Trust management approach will aid in monitoring the network interactions in a more secure way thus creating a safer environment given the potential availability of different threats in the field. The initial idea of a behavioral-based model was developed, which expanded upon traditional trust management to aid in the real-time detection and mitigation of threats. The development of a behavioral-based trust management model offers further protections in an IoT environment as it can detect and mitigate threats in real-time. Further, this can aid in traditional trust management approaches through the inclusion of a behavioral value to allow for a more accurate measurement of trust.

Blockchain can provide a distributed database that can support that whole network where entities can contribute to it with the ability to monitor any misreporting information that is supported by the tamper proof capability of Blockchain. This makes Blockchain a great tool to support a global view of the network where sharing information between entities is a must. This design can be applied to different applications related to smart cities to ensure the data being shared is tampered proof, where any entity in the system has the ability to verify the entry, such as smart homes, smart traffic lights, and traffic violation reporting systems.

Scholarly Products

Publications:

1. F. Kandah, B. Huber, A. Altarawneh, S. Medury and A. Skjellum, "BLAST: Blockchain-based Trust Management in Smart Cities and Connected Vehicles Setup," 2019 IEEE High Performance Extreme Computing Conference (HPEC), Waltham, MA, USA, 2019, pp. 1-7, doi: 10.1109/HPEC.2019.8916229.
2. F. Kandah, A. Altarawneh, B. Huber, A. Skjellum, and S. Medury, "A Human-Understandable, Behavior-based Trust Management Approach for IoT/CPS at Scale," Int. J. of International Society for Computers and Their Applications (ISCA), In Press (2020)
3. J. Coleman, F. Kandah and B. Huber, "Behavioral Model Anomaly Detection in Automatic Identification Systems (AIS)," 2020 10th Annual Computing and Communication Workshop and Conference (CCWC), Las Vegas, NV, USA, 2020, pp. 0481-0487, doi: 10.1109/CCWC47524.2020.9031248.
4. A. Altarawneh, T. Herschberg, S. Medury, F. Kandah and A. Skjellum, "Buterin's Scalability Trilemma viewed through a State-change-based Classification for Common Consensus Algorithms," 2020 10th Annual Computing and Communication Workshop and Conference (CCWC), Las Vegas, NV, USA, 2020, pp. 0727-0736, doi: 10.1109/CCWC47524.2020.9031204.

External Conferences:

1. IEEE High Performance Extreme Computing Conference (HPEC)
2. IEEE 9th Annual Computing and Communication Workshop and Conference (CCWC)

Presentations at UTC:

1. The plan was to present part of the work developed in this project in the UTC Research Dialogue, but due to Covid-19 restrictions the conference was canceled.

Inventions or Other Intellectual Property

N/A. But very interested to explore and learn about the invention disclosure/commercialization process.

Research Outreach & Collaboration

- IMSA
- EPB
- Auburn University
- Tennessee Tech University
- Middle Tennessee State University

EXTERNAL FUNDING

Proposal Submissions

1. NSF EAGER
2. NSF SaTC
3. NSF CCRI

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

A number of meetings were held with the grant administrator at SimCenter in support of our ongoing proposal. These meetings included reviewing our proposal, providing guidance and directions which were very beneficial in creating a well written proposal.

The graphic designed personnel was very helpful at different occasions during the development of our external proposals.

WHAT'S NEXT FOR THIS RESEARCH?

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

As IoT systems become a part of our daily lives, our plan is to extend this research and explore different areas that can benefit from this work especially in investigating different setups such as static networks (Smart home), dynamic networks (Connected vehicles) and hybrid networks to include both static and dynamic. As we continue evaluating and testing Blockchain setups, we will continue our work to support Blockchain-based applications and ensure their applicability in small IoT devices.

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

We would like to explore and investigate more into the machine learning area and how it can benefit our trust management algorithms. Also, we would like to investigate the design of smart cities and what is the optimal approach to off load any computational overhead occurring in the system to more resourceful devices while maintaining the dynamicity and the real-time factors to support smart cities' setups.

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?

To develop the required Blockchain testbed, there is a need to access the labs and work with the equipment to be able to design the testbed and be able to connect the devices together and test/evaluate the system on a larger scale. This might be limited due to the Covid-19 restrictions across campus.

FINANCIAL ACCOUNTING

Due to the restrictions that occurred at the last quarter of the project caused by Covid-19, there are a number of activities that were not possible such as travel and conference attending which were budgeted for but couldn't be spent.

Fiscal Year 2020 Final Project Report

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

Francesca Leasi, Lead PI

Co-PI(s): Bathi J.; Gao C.; Qin H.
Other Personnel: N/A

Project Title: “Simulating bio-environmental interactions using –omics approaches”

Date Submitted: 02/27/2018

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

Non-Technical Summary:

The primary objective of this project was to simulate pollution load from point and non-point sources in urban watersheds. While the proposed task of the project is to simulate North Chickamauga Creek watershed, in co-ordination with our efforts on other CEACSE project, we also worked to develop South Chickamauga Creek watershed. Both the watersheds are delineated using ArcGIS, and other relevant data for the watershed model set-up is processed using Environmental Protection Agency (EPA) BASINS 4.5. Calibration of these parameters is always challenging due to limited access to the observed water quality data. However, to make a satisfactory fit with USGS observed water quality data, we gathered information of the location of point sources within the watershed and now we are underway of adding the point sources data into the model. From the same locations, biological data were obtained using environmental DNA approaches. Data of different nature will be joined to understand correlations between hydrogeology dynamics and biodiversity.

Results were presented in five conferences; one manuscript is currently under preparation. Two graduate students worked on the project and more undergraduates will work next year thanks to possibility to carry over part of the budget.

PROJECT TITLE: Simulating bio-environmental interactions using –omics approaches
Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
• Develop watershed model • Obtain e-DNA information • Correlate information obtained by the two disciplines	Both the watersheds are delineated using ArcGIS, and other relevant data for the watershed model set-up is processed using Environmental Protection Agency (EPA) BASINS 4.5. To address Spatial variation in land use and surface imperviousness each watershed was divided into a number of sub-watersheds. After completion of watershed delineation, the files from BASINS were put into the Hydrologic Simulation Program FORTRAN (HSPF). HSPF is an equivalent model to Storm Water Management Model (SWMM) proposed in initial proposal and is capable of providing very same parameter information as SWMM. In HSPF, every sub-watershed gets connected with its upstream and downstream sub-watersheds according to the stream links (i. e. direction of flow). During the set-up process, the HSPF model incorporates major sources of flow and water quality loads into the simulation. NLCD 2016 land cover and NLCD 2016 percent imperviousness (CONUS) were used to address land use and surface imperviousness of the watershed and corresponding values are assigned by sub-basins in the HSPF model. Meteorological data was collected from North American Land Assimilation System (NLDAS) which provides all necessary meteorological parameters. However, the potential evapotranspiration values were estimated using Hamon PEVT and using a multiplier the results were matched with the long-term Free Water Surface (FWS) Evaporation described in the hydrologic document NOAA Technical Report NWS 33. Simulated results of daily flow along stream reaches was calibrated against the United States Geological Survey (USGS) monitored stream flow for the period of 2013 – 2016 and validated for the year 2017. In the

	process of calibration parameters like length of overland flow and slope of overland plane were measured using ArcGIS. Soil infiltration parameters were tuned based on the soil and land use category of each watershed. Also, several parameters like upper and lower zone storage nominal, interflow and ground water parameters, monthly storage capacity, manning's co-efficient etc. were selected according to the land use, soil, and runoff characteristics of the study area. Simulated annual flows from the calibrated model were kept within 10% of the observed flows from the USGS monitored gages. In addition to daily discharge, HSPF model predicted water quality parameters such as dissolved oxygen (DO), biochemical oxygen demand (BOD), nutrients, sediments, water temperature, phytoplankton, etc. for a continuous time series of meteorological parameters. Calibration of these parameters is always challenging due to limited access to the observed water quality data. However, to make a satisfactory fit with USGS observed water quality data, we gathered information of the location of point sources within the watershed and now we are underway of adding the point sources data into the model.
RESULTS	**OTHER INFO**
	Budget and Schedule Total Budget: $100,000 Actual Used: $90,000 Balance: $ 10,000 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-6 Task 3: Months 6-12 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved.

	• Final report detailing results, financials, and future work • Publication • External and internal conference presentation **Organization Information** Department of Biology, Geology and Environmental Science UTC

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Watershed models	- Specific points to start sampling environmental DNA have been assessed. - An initial skeleton of the numerical hydrology model has been setup successfully. - Both the watersheds are delineated using ArcGIS, and other relevant data for the watershed model set-up is processed using Environmental Protection Agency (EPA)
e-DNA	- Sample collected - Preliminary data obtained - More data in 2020-21
-statistical correlations	- need to be done after all data is available. It will be mostly done in 2021.

Challenges & Strategies Used to Address / Overcome:

The project was probably too ambitious to be completed in one year. There were several impediments, including a water flooding in the PI's lab, which prevents her to obtain data. The first year has focused on the development of the watershed model. The carryover (due to COVID-19) will be used to obtain more biological data in the second year.

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 data of this project allowed me to submit an NSF proposal in 2019. The proposal didn't get funded. However, the process has been extremely useful to prepare a second proposal, which has been submitted to the NSF CAREER program in 2020.

Students Impacted

Preyanka Dey. MA. Civil Engineering Department. She has been completely supported by CEACSE grant. Next year, she will be supported by Dr. Hope Klug and continue working on the watershed model.

Adrianna Hodges. MA. in Environmental Science Department. She was partially supported by CEACSE as she obtained a Teaching Assistantship from the BGES Department. Unfortunately,

the collaboration did not work out and she stopped being supported a few months into the project. The carryover will be used to support undergraduates in biology, who will continue obtaining data.

Community and Broader Impacts

N/A

Scholarly Products

Publications:

Preyanka Dey, Jejal Reddy Bathi, Francesca Leasi, “Sensitivity of HSPF Model watershed hydrology for BASINS 4.5 Land Cover and Meteorological Databases” (manuscript under preparation)

External Conferences:

Preyanka Dey, Jejal Reddy Bathi, “Watershed modeling techniques to understand impacts of pollutants on microbiology”, EWRI Watershed Management Conference 2020, Henderson, Nevada, May 17- May 21, 2020. (Poster Presentation)

Preyanka Dey, Jejal Reddy Bathi, Francesca Leasi “Hydrologic models to evaluate pollutant's impacts on microbiology”, Tennessee Water Resource Symposium, Montgomery Bell State Park, Burns, TN, April 22 – 24, 2020.

Preyanka Dey, Jejal Reddy Bathi “Hydrological Modeling for Watershed Management, Technology Symposium”, Downtown Library, Chattanooga, Tennessee, April 17, 2020.

Preyanka Dey, Jejal Reddy Bathi, Francesca Leasi “Hydrological Modeling of South Chickamauga Creek watershed using BASINS/HSPF”, TNSA Annual Conference Going the Distance in 2020. (Podium presentation)

Presentations at UTC:

Preyanka Dey, Jejal Reddy Bathi, Francesca Leasi “Urban water resources management using BASINS/HSPF”, University of Tennessee RESEARCH Dialogues, April 15, 2020.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

N/A

EXTERNAL FUNDING

Proposal Submissions

1. 2020. Ruth S. Holmberg Grants for Faculty Excellence. University of Tennessee at Chattanooga. Funded

2. 2020. Faculty Achievement Award. College of Arts & Sciences. University of Tennessee at Chattanooga. Funded
3. 2020. NSF CAREER Program – Division of Environmental Biology. Under Review
4. 2019. NSF– Division of Environmental Biology. Declined
5. 2019. NSF – MRI. Declined

Contracts/Awards Received

1. 2020. $4,800. PI. “Biodiversity of Microscopic Invertebrates in Hamilton County Using Cutting-edge Molecular Approaches”. Ruth S. Holmberg Grants for Faculty Excellence. University of Tennessee at Chattanooga.
2. 2020. $1,000. PI. “Smithsonian Marine Station (SMS) Meiofauna Diversity and Taxonomy Workshop”. Faculty Achievement Award. College of Arts & Sciences. University of Tennessee at Chattanooga.

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 have recently received a Ruth S. Holmberg Grants for Faculty Excellence Award, which project focuses on similar aspects of the CEACSE grant. My plan is continue working on the biodiversity of Hamilton County and obtain more data, properly analyzed, to be used as preliminary data for future NSF grants. I also plan to establish collaborations with local agencies.

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

I will submit another NSF grant but only after solid preliminary data will be achieved.

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

Fiscal Year 2020 Final Project Report

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

Dr. Eleni Panagiotou, Lead PI

Co-PI(s): Jin Wang, Abi Arabshahi, W. Y. Yang, Chris Dowell
Other Personnel: Evan Gildernew

Project Title: Polymer Entanglement

Date Submitted: 02/27/2017

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

Non-Technical Summary:

This proposed research is focused on making the connection between microscopic and macroscopic properties in polymers and biopolymers. Our Objectives were to (1) link viscoelastic properties with polymer entanglement (2) use the partitioned model simulation of polymers in order to account for fluid-structure interactions and (3) experimental study of RNA to understand the relation between topology and biological function. Our outcomes showed (1) a direct relation between the periodic linking number and the molecular weight of polymers, while the viscoelastic response varied from the Rouse to the entangled regime (2) the flattening of polymer knots/links in Couette flow, depending on the knot/link type (3) the geometry of binders to RNA repeats related to disease share a similar pattern compared to non-binders. (1) contributes to the field of Chemical Engineering, Polymer Physics and Mathematics by providing rigorous relations between polymer characteristics and their topology, (2) contributes to the field of Chemical Engineering, Polymer Physics and Mathematics by providing rigorous relations between fluid flow of polymeric solvents and their topology, (3) contributes to the field of Biology and Mathematics by providing a novel approach to detect binders to specific RNA sequences. During this time 3 papers and 8 presentations were published by E. Panagiotou, E. Gildernew was supported by the grant and presented his results in a poster at UTC Research Dialogues, while the PI also mentored 1 undergraduate student in Mathematics who was supported by the grant. J. Wang gave 1 talk, Y. W. Yong gave 1 presentation at a conference and mentored 2 undergraduate students supported by the grant. A. Arabshahi contributed research advice and expertise to the broader SimCenter infrastructure and C. Dowell contributed technical support in installing LAMMPS at the SimCenter computers and the cluster. E. Panagiotou and Jin Wang were awarded an NSF grant ($125,000). E. Panagiotou has also applied for an NSF:MODULUS grant, which is still pending. This project advanced or supported the mission of the SimCenter by obtaining external funding, by publishing to peer-reviewed scientific journals and conferences where the SimCenter is mentioned and by training students.

PROJECT TITLE: A study on the local and global effects of polymer entanglement in material properties and biological functions
Technology Area of Interest: ADVANCED MODELING AND SIMULATION

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

RESULTS	**OTHER INFO**
	Budget and Schedule Total Budget: $ 99,941 Actual Used: $71,211 Balance: $ 28,729 Total period of performance is 12 months. Task 1: Months 1-6 Task 2: Months 3-6 Task 3: Months 6-12 Task 3: Months 8-12 **Deliverables** • Monthly report describing numerical methods, techniques, and results that were developed or improved. • Final report detailing results, financials, and future work • Publications(papers and presentations) • External and internal conference presentations **Organization Information** *SimCenter, University of Tennessee at Chattanooga, eleni-panagiotou@utc.edu*

ACCOMPLISHMENTS & OUTCOMES

Project Overview

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

(1) The Molecular Dynamics (MD) simulation of polymers and biopolymers and their topological analysis.

(2) The partitioned model simulation of polymers and biopolymers in order to account for fluid-structure interactions.

(3) The experimental study of RNA polymeric systems in order to study their relation to polymer mechanics and function.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
MD simulations of varying molecular weight polymer melts in an oscillatory shear experiment	Completion of initial simulations, results presented in UTC Research Dialogues
Topological analysis of MD simulation results	Preliminary results obtained, working on the completion and on a manuscript (continuing work with PI and Evan Gildernew)
FSI simulations	Completion of simulation settings that can handle the FSI simulation of polymers (continuing work with J. Wang and J. Gounley-ORNL)
RNA repeats and binder analysis	Preliminary results suggest further analysis is needed.
MD simulations of RNA repeats	Was not accomplished
New measures of topological entanglement	Creation of the Jones polynomial of open chains and creation of computational code in python

Challenges & Strategies Used to Address / Overcome:

We were not able to begin the MD simulations of RNA. The reason for this was the preliminary results on RNA and binder topological analysis took longer than expected, because it was difficult to obtain the experimental binder and non-binder molecules. In order to overcome this problem, one more graduate student would be required to work on the project with focus on Molecular Simulation. In order to attract and train such students, the PI is planning to 1. Teach a course on Applied Knot Theory in Fall 2020 and 2. Plan to teach a course on Molecular

Simulation (possibly for Spring 2020). Students who take those courses will be ready to actively participate and contribute to various research projects.

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

The MD simulations of RNA repeats were not completed. A reason for this was that the graduate students training took longer than expected. I trained a student for 4 months at the Department of Mathematics, but realized that he was not a good fit for the research, despite this effort. For this reason, I took an alternative approach which used the optimized structures of binders to RNA instead of MD obtained structures. (This proved to be a beneficial idea in other contexts which I am already working on and led to a part of a project related to COVID19). The results on binder molecules to RNA so far are inconclusive but not negative. A reason for this is that we need more data. The data were obtained by co-PI Y. W. Yong by using an online software for obtaining optimized 3-D structures of binder molecules. This process was much slower than expected. There are two reasons for this: 1. Not having free access to the gaussian program, 2. Not having a student to work on this. From that I learned that it would be important to obtain a free access to the Gaussian program and train students in Chemistry to using such Chemical computational packages.

IMPACT & OUTCOMES

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

The PI had the chance to advise 1 graduate student in Chemical Engineering and 1 undergraduate student in Mathematics. Also, she conducted research and published her work in peer-reviewed journals and in conferences and seminars. The PI and co-PI Jin Wang submitted and were awarded an NSF grant to work on this topic. The PI applied for a grant on the topology of protein folding, NSF: MODULUS which is pending. She also applied for other external funding that was not awarded. The PI is now preparing her second application for an NSF CAREER grant and all this has been very beneficial. The PI and co-PI Jin Wang established a new collaboration with ORNL in the framework of this grant.

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

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

The co-PI Y. W Yong had the chance to advise 2 undergraduate students.

Students Impacted

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

Peter Zeglen, participated in research, graduated Bachelor in Mathematics

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

Matthew Phanner, participating in research, Bachelor in Chemistry

Justin Pease, participating in research, Bacelor in Chemistry

Community and Broader Impacts

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

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

Scholarly Products

Publications: All publications were in peer-reviewed scientific journals

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

External Conferences:

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

The PI was planned to present the results in the following meetings which were canceled due to COVID19:

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

Presentations at UTC:

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

Inventions or Other Intellectual Property

N/A.

Research Outreach & Collaboration

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

A new collaboration was created with the PI, Jin Wang and John Gounley from ORNL. The framework for FSI simulations has been created and tested for certain topologies. We are now working on the derivation of the key topologies that will enable us to detect the effects of entanglement in FSI in larger scale simulations.

The PI was planning to host high-school students in UTC (on campus) for a day (cancelled due to COVID19).

EXTERNAL FUNDING

Proposal Submissions

1. NSF Proposal on Entanglement in Polymers submitted prior to reporting period but immediately related to the proposed work.
2. NSF CAREER: Topology of the cytoskeleton (not funded)
3. NSF MODULUS (pending)

4. ORAU Powe award (pending)

Contracts/Awards Received

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

Sponsored Program Capacity Building Activities

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

WHAT'S NEXT FOR THIS RESEARCH?

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

In the next year the PI will continue working with E. Gildernew towards the completion of a paper that will be submitted for publication. The PI and co-PI Jin Wang will continue working with John Gounley ORNL on the FSI simulations of polymers. These results will shed light in the very complex relation between entanglement and fluid flow. Our results will lead to papers and possibly to new applications for external funding. The PI will continue working on using topology to finding binders to RNA repeats, but also in another direction: She has established a collaboration with Bobby Sumpter, ORNL and she studies binders to the Spike protein of COVID-19. The PI will apply for an NSF CAREER award in August 2020. The PI will also continue her research in creating new measures of topological entanglement which may lead to a new application to NSF DMS. The PI applied and obtained funding for organizing an international meeting at the Banff International Research Station in June 2021.

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 ORN 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.

None.

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

An important barrier is the lack of interested graduate students. I have had difficulty in finding students that can contribute to the Mathematical research and would wish to support students from Mathematics. I hope that the new course Applied Knot Theory will attract interested students in applied Mathematics who will participate in research. Also, I hope that the AMS meeting that will be held in Fall 2020 and the meeting in BIRS in summer 2021 will attract more interested students in research at UTC.

FINANCIAL ACCOUNTING

Due to COVID-19, $10,000 for supporting students were carried over.

Fiscal Year 2020 Final Project Report

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

Dr. Jared A. Pienkos, Lead PI

Co-PI(s): Dr. Wang-Yong Yang and Dr. John P. Lee
Other Personnel: Dr. Colin McMillen (Collaborator, Clemson University), Dr. James Burgess (Collaborator, JASCO), Dr. Paul S. Wagenknecht (Collaborator, Furman University), Dr. Berhane Temelso (Collaborator; formerly College of Charleston, now George Mason University), Tracie Durham (Girls Preparatory School).

Project Title: "Alkynyl tetrafluoro-pyridyl ligands: computational studies, synthesis, and characterization"

Date Submitted: 02/27/2017

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

Non-Technical Summary:

From this funding, the PI and Co-PI(s) were able to train nine undergraduate research students. Their work resulted in the submission of two manuscripts, one accepted (https://doi.org/10.1016/j.inoche.2019.107722), and the others under review. Both manuscripts involved the PI's collaborator at Clemson University, and the manuscript under revision involved the PI's collaborator at College of Charleston. This opportunity allowed us to establish a collaboration with James Burgess (JASCO), and we are currently working on another publication (Tuning the Optical and Electrochemical Properties of Transition Metal Compounds Containing and Ethynyl Pyrimidine Ligand). During this time the PI also started a new project with Paul Wagenknecht (We will likely submit a publication in the near future).

The funding allotted in this grant allowed us to synthesize a variety of compounds with novel structural and optical properties. Using the TS cluster at the Sim Center, we were better able to characterize these compounds with computational chemistry. We hope to continue running calculations using the resources of the Sim Center.

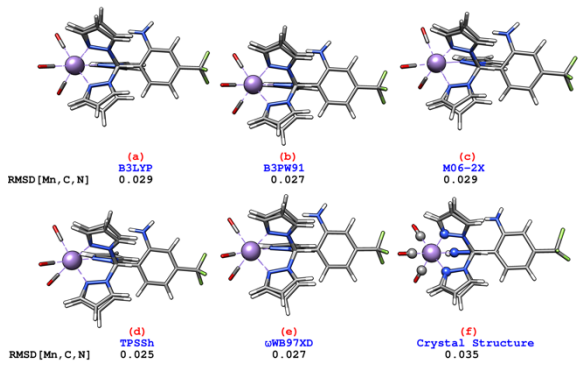
PROJECT TITLE: Alkynyl tetrafluoro-pyridyl ligands: computational studies, synthesis, and characterization

Technology Area of Interest: Health & Biological Systems

TECHNICAL APPROACH	OUTCOMES
1) Synthesize compounds with novel optical and structural properties. Fully characterize these compounds, including techniques involving computational methods. 2) Continue outreach program through computational modeling demonstrations and interactions with the community.	1) We were able to generate a variety of compounds with novel structural and optical properties-two publications submitted through this endeavor. 2) We were able to perform three outreach activities, we mentored one high school student (she will be a co-author on a future publication), and we established a new collaboration with James Burgess (JASCO)

RESULTS

An example result is shown below. Synthetically we were able to generate new ligands, and characterize these compounds through X-Ray crystallography with the help of Colin McMillen. Using computational modeling, with the help of Berhane Temelso, we were able to compare how different levels of theory predicted our structures (The newly submitted publication is attached, SI1 and SI2). To quickly and efficiently do this type of modeling HPC resources are necessary.



OTHER INFO

Fill in your info below.

Budget and Schedule

Total Budget:	$74,832.00
Actual Used:	$67,279.00
Balance:	$ 6,552.49

Deliverables

- Two publications were submitted

Organization Information

Jared Pienkos

320 Grote Hall, Dept 2252, 615 McCallie Ave, Chattanooga, TN 37403.

732-513-2644, Jared-pienkos@utc.edu

ACCOMPLISHMENTS & OUTCOMES

Project Overview

During the course of this project period, we designed and characterized emissive transition metal complexes, namely ^{t}bpyPt(C_2pym)$_2$ and $PPh_3Au(C_2pym)$. A main focus of our research was to design compounds that have blue shifted (high energy) emission. We originally planned on only focusing on platinum derivatives; however, we found that gold compounds with emissive properties could be easily synthesized (Figure 1). The ^{t}bpyPt(C_2pym)$_2$ is a slight deviation from our original synthetic target ^{t}bpyPt(C2py^{F})$_2$. Unfortunately, because Furman University shut down, we were not able to rigorously characterize these compounds spectroscopically. Fortunately, working with our collaborator from JASCO, we were able to electrochemically demonstrate these compounds will be excellent emitters, and will have a blue shifted emission compared to a commonly studied platinum derivative ^{t}bpyPt(C_2Ph)$_2$. We were also able to show this computationally by performing electronic structure calculations.

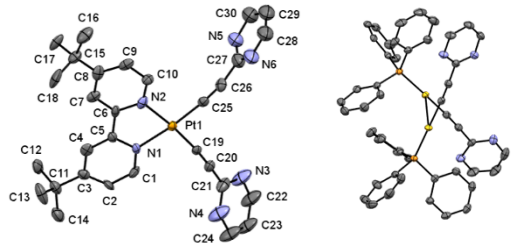


Figure 1: Emissive Platinum (left) and gold (right) complexes.

Working with our collaborator from college of Charleston, we learned how to model transition metal compounds and determine what levels of computational theory produced the best structural comparisons (Figure 2). We are also performing this type of analysis with the platinum and gold species. In computational chemistry, it is important to perform these benchmark studies. For instance, once we perform this type of benchmark study on ^{t}bpyPt(C_2pym)$_2$, we will be better able to model ^{t}bpyPt(C_2py^{F})$_2$ once it's synthesized.

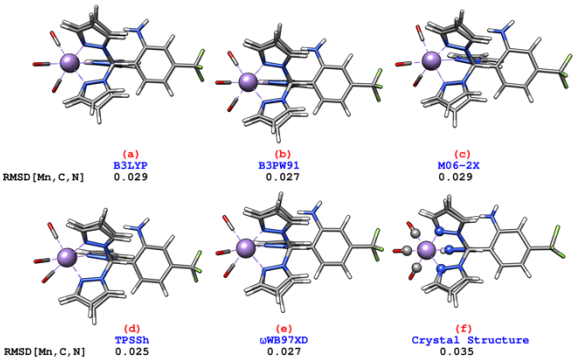


Figure 2: Overlay of DFT/6-311++G(d,p) calculated [H_2NPh(CF_3)(CPz_3)Mn(CO)$_3$]+ and [TpmMn(CO)$_3$]+ structures.

Another platinum derivative we investigated during the course of this study was ^{Ph}bpyPt(C_2CF_3)$_2$. We worked with Furman university to develop models for this system. Initial goal was to generate a crystal structure of this compound. From crystal structure data, we can generate coordinates of atoms that we can then import into modeling software. Unfortunately, we were not able to get our intended compound ^{Ph}bpyPt(C_2CF_3)$_2$ to crystalize out of solution. Instead, we crystalized an impurity (Figure 3).

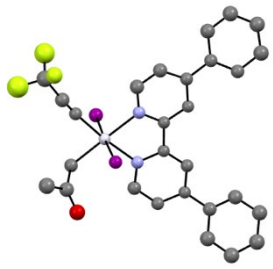


Figure 3: Impurity generate from crystallization.

Within the year, we will publish our work investigating the ^{t}bpyPt(C_2pym)$_2$ and $PPh_3Au(C_2pym)$ species, which will demonstrate the utility of pyrimidine ligands to tune the photophysical properties of metal systems.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Submit 2 Proposals	Submitted ACS PRF Proposal and NSF REU Proposal (will submit NSF-Career)
Train Students	Seven undergraduate students were trained using the resources of this funding. One High School student was trained
Perform outreach activities	Three outreach activities were performed
Develop Collaborations	New collaboration established with JASCO
Submit Manuscripts	Two manuscripts were submitted. We are drafting two manuscripts (maybe 3) based on the results of this proposal.

Challenges & Strategies Used to Address / Overcome:

We struggled with our original synthetic target. Initially, we planned on making a ligand (compound that binds to a metal) to tune how a metal emits light. We found the ligand synthesis extremely difficult. Fortunately, we discovered a commercially available compound that hasn't been utilized to transform the optical properties of transition metal compounds. We utilized this compound to generate emissive gold and platinum compounds. We plan on publishing an in depth report on the use of this ligand within the next year.

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

We are still working our original ligand target (see above). We also were not able to examine how secondary site interactions affected the optical properties of transition metal complexes. From performing more in depth literature reviews, we found this concept, while not overly explored, may not be worth pursuing because more novel means of tuning the optical properties of transition metals are available. Future work will focus on examining halogen-bonding to change the optical properties of transition metal complexes.

IMPACT & OUTCOMES

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

The PI was able to train nine undergraduate students, publish, and develop new ideas that he'll carry out with his collaborators. Of note, one of the collaborators, John Lee, will write an NSF REU grant based on a "spin-off" project generated during this project. Two of the eight research students were able to run an outreach program using web-based computational chemistry.

Students Impacted

1) Hailey Beaver, a biology major (Class of 2022). She plans on attending medical school.

2) Sarah McDarmont, a chemistry major (Class of 2021). She plans on attending graduate school.

3) Sophia Neglia, a chemistry major (Class of 2021). She plans on attending graduate school.

4) Logan Jaques, a chemistry major (Class of 2021). He plans on attending graduate school or getting a job at a chemical company.

5) Anastasia McConkey, a chemistry major (Class of 2020). Received a job at New Blooms Laboratory.

6) Tiffany Truong, a chemistry major (Class of 2022). She plans on attending graduate school.

7) Zach Moser, a chemistry major (Class of 2020). Received a job at Aegis.

8) Jasmine Suggs, a chemistry major (Class of 2020). Look for an industrial chemistry job.

9) Brandon Nessell research, a chemistry major (Class of 2022). He plans on attending graduate school.

Community and Broader Impacts

We performed three community outreach activities that center around browser based computational chemistry. We will continue these types of activities following the funding period.

Scholarly Products

Publications:

Undergraduate mentees underlined.

1. Jaques, L. D.*; McDarmont, S. L.*; Smart, M. M.; McMillen, C. D.; Neglia, S. E.*; Lee, J. P.; Pienkos, J. A., Structural characterization of the metalloligand tbpyPt(C22-py)2 and its interaction with Pd(OAc)2. *Inorganic Chemistry Communications* 2020, 112, 107722. (IF 1.943)

Pienkos, J.A., Exploiting a C-F activation Strategy to Generate Novel Tris(pyrazolyl)methane Ligands (submitted ZAAC, IF 1.24)

External Conferences:

Undergraduate mentees underlined.

1. Neglia, S.*; Lee, J. P.; Pienkos, J. A. Synthesis, characterization, and reactivity of a heterobimetallic organometallic complex with a trans bidentate ligand for catalytic carbon-hydrogen bond activation. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

2. Truong, T. T.*; Mconkey, A. M.*; Moser, Z. D.*; McDarmont, S. L.*; Lee, J. P.; Wang-Yong, Y.; Pienkos, J. A. Synthetic strategies for generating 4-ethynyl-2,3,5,6-tetrafluoropyridine. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

3. Jaques, L. D.*; McDarmont, S. L.*; McMillen, C.; Neglia, S.*; Lee, J. P.; Pienkos, J. A. Synthesis of tbpyPt(C22py)2 and its interactions with Cu(I) and Pd(II) metals. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

4. McDarmont, S. L.*; Jaques, L. D.* Synthesis of multi-metallic acetylide compounds of d10 transition metals. Abstracts, 71st Southeastern Regional Meeting of the American Chemical Society, Savannah, GA.

Presentations at UTC:

N/A

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

We will continue working with Colin McMillen (Collaborator, Clemson University), James Burgess (Collaborator, JASCO), Paul S. Wagenknecht (Collaborator, Furman University), Berhane Temelso (Collaborator formally, College of Charleston, now, George Mason University), and Tracie Durham (Girls Preparatory School).

EXTERNAL FUNDING

Proposal Submissions

1. ACS PRF- Exploiting Metallohinged *Trans*-bidentate Ligands for Suzuki Coupling

2. NSF REU- Exploiting Pyridyl-based Ligands and Secondary Site Interactions in Transition Metal Alkynyl Compounds

3. NSF Career- Exploiting Halogen-Bonding to Tune to Optical Properties of Transition Metals for Their Use in Organic Light Emitting Diodes.

Contracts/Awards Received

1. N/A

My research student receive the Inspiring Women in Lifelong Leadership (I WILL) Award for mentoring a high school student.

Sponsored Program Capacity Building Activities

1. 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?

1-2 years-We hope to have two more publications from this work. We will include our new collaborator from JASCO. We will present this work at a national meeting.

After 2 years-we believe the synthetic methodology investigated in this work will allow us to generate materials that exploit halogen-bonded networks to produce novel optical materials (https://doi.org/10.1016/j.ccr.2019.213107). Working with our computational collaborator, we hope to develop techniques to model these systems.

The PI will submit at least one proposal per year based on the preliminary research performed during this grant period.

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

We will collaboration with Clemson University, Furman University, Jasco, and Girls Preparatory School. The PI will also begin a project Sungwoo Yang (Chemical Engineering Department). The synthetic methodology developed from this proposal will be beneficial for this collaboration.

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?

Some licenses for computational software will expire in the near future. While the PI is happy to pay for these costs (around $1000/year) with grant money, if the PI does not receive any external funding these licenses may not be renewed.

FINANCIAL ACCOUNTING

We have not spent the full amount of the grant. Some of the funds were intended for carryover to support student research and travel. These values may need to be adjusted because we overspent the materials & supply line of the budget. Please contact Michelle Walters with any questions (michelle-walters@utc.edu).

Fiscal Year 2020 Final Project Report

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

Dr. Sungwoo Yang, Lead PI

Project Title: “Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling”

Date Submitted: 07/31/2020

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

Non-Technical Summary:

Access to clean water is one of the largest challenges that we face in the world today. We proposed water harvesting from ambient air by adsorption with advanced porous zeolites (ZT). During operation, ZT particles are exposed to ambient air, during which the water vapor (humidity) is adsorbed. To harvest the adsorbed water from zeolites, low-grade heat (below 100 °C), such as solar thermal energy, can release the water for condensation and collection. Here, with commercially available advanced zeolite as adsorbents, we leverage our development of light-weight carbon network as thermal additive and computational analysis to obtain an efficient design for water harvesting. As a result, our novel approach can achieve effective and efficient water harvesting, with a >2.5x higher energy efficiency compared to commercial atmospheric water generators (AWGs).

We developed flexible 3-dimensional carbon network (3dCN) to maximize gravimetric and volumetric water harvesting due to its lightweight, flexibility and high thermal conductivity. On the other hand, to optimize the performance of AWGs, we have developed Finite Element (FE) model that considers coupled mixed solver dimensionalized by Rayleigh, Horton Rogers Lapwood, heat transfer, and topical optimization. Molecular dynamics modeling is also studied using LAMMPS. The works has progressed on innovative material (3dCN), Python codes, and techniques for engineering nanofluidic materials. 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 under ambient conditions to demonstrate the viability of this approach. With preliminary data and modeling results mentioned above, 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: Optimization of Sunlight Powered Water Harvesting from Air by Characterization and Modeling
Technology Area of Interest: Energy Thrust

TECHNICAL APPROACH	OUTCOMES
The major milestones include 1. Fabrication of 3dCN / ZT adsorption layers 2. Computational device design optimization 3. Devices testing with a dynamic adsorption system	The research outcomes include 1. Submitted a proposal, $1.4M, (concept paper) for the DARPA call on Atmospheric Water Extraction (AWE, HR001120S0014), but not selected. 2. In progress (~65%), a peer-reviewed publication on AWE modeling 3. In progress (~50%), a peer-reviewed publication on an innovative 3dCN as lightweight and flexible thermal additive
RESULTS	**OTHER INFO**
Please, see the attached research report for the details	**Budget and Schedule** Total Budget: $99,959.00 Actual Used: $98,551.00 Balance: $ 1,408.00 **Deliverables** • External funding proposal (submitted) • Monthly report describing numerical methods, techniques, and results that were developed or improved. (submitted) • Final report detailing results, financials, and future work (submitted) • Publication (in progress) • External and internal conference presentation (delayed due to COVID-19)

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Fabrication of 3dCN	Completed. In progress, for a publication
Fabrication of 3dCN/ZT adsorption composite	Fabricated. In progress for more characterization
Computational device design optimization	FEM model developed. In progress, for multiple publications
Building a dynamic adsorption system	Delayed due to COVID-19. But materials-level characterization instrument purchased to continue the project

Challenges & Strategies Used to Address / Overcome:

Followed are the challenges and strategies associated with the proposed project:

1. Laboratory space: a chemical vapor deposit (CVD) system to synthesize 3d-CNT requires exhaust system. Dr. Yang's lab (EMCS 214C) currently does not have exhaust system yet. → To resolve the issue, a CVD system has been installed in the chemical engineering lab (EMCS 120) to utilize the existing exhaust system.
2. International chemicals: foresaid advanced zeolite (AQSOA, Mitsubishi) is located in Japan. Currently, 3 kg of the advanced zeoltie is avaialbe at UTC. Additional international purchase might include few unexpected issues. → The chemical was purchased succefully.
3. Limited researcher power: the proposed project requires significant amont of efforts to conduct various experiments and theoritical modeling. → Limited researcher power was major challenge the PI has been facing. Especially, due to COVID-19, it was extremely difficulty to keep researchers. As results, the several milestones were delayed, but the PI continue to work on the project to produce research publications and external funding. The PI will keep looking for hiring student researchers for upcoming semesters.

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

We have achieved noticeable research results on fabricating an innovative 3dCN thermal additive and on development of computational modeling. However, we were not able to build a device-level dynamic adsorption system, mainly due to limited researcher power. The PI plan to utilize the material-level characterization instrument (DVS adsorption, purchased by the CEACSE fund) to continue the project. We plan to build a device-level dynamic adsorption system later once we confirm promising research results.

IMPACT & OUTCOMES

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

With preliminary data and modeling results mentioned above, the PI plans to pursue external funding opportunities related on water harvesting applications including NSF, NASA, ARPA-e, DARPA and etc. In addition, in a collaboration with Dr. Dion Antao at Texas A&M University, the PI plans to submit a proposal seeking an external funding opportunity at Office of Naval Research (ONR). External funding awards would demonstrate prior success and serve to strengthen an NSF CAREER proposal by the PI.

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 is now considering to pursue Ph.D. program at UTC.

Emily Chase (JGJ444, 2020 graduated) was an undergraduate student who has been working on the synthesis of 3dCN for a year. She found interests in research, and join Northwestern University to purse her Ph.D. in Chemical Engineering.

The PI found a computational research group, and multiple undergraduate students joined the group including Jasper Emerton (MXW171), Alex Rutter (FRX829), Erik Loredo (GCL841) and John Roberts (JJF842). They are eager to learn about Python and FeniCS.

Community and Broader Impacts

No community impacts have been made yet, but the PI is looking forward to working with local companies and organizations who are interested with the water harvesting applications.

In addition, with the computational modeling experience, the PI creates a graduate level course, ENCH 5910R Molecular Dynamics Simulations.

Scholarly Products

Publications:

1. Thermal and Mechanical Properties of 3-Dimensional Carbon Network as Flexible Thermal Additives (in progress, 50%)
2. Optimization of The Adsorbent Geometries of Water Harvesting System by Finite Element Method (in progress, 65%)

External Conferences:

Delayed due to COVID-19

Presentations at UTC:

Delayed due to COVID-19

Inventions or Other Intellectual Property

No patent application has been submitted yet, but the PI plan to submit one if applicable in the near future.

Research Outreach & Collaboration

The PI joins SimCenter affiliation with Energy Thrust to promote collaboration seeking external funding opportunities.

EXTERNAL FUNDING

Proposal Submissions

1. Submitted a proposal, $1.4M, (concept paper) for the DARPA call on Atmospheric Water Extraction (AWE, HR001120S0014), but not selected.

Contracts/Awards Received

Nothing available yet.

Sponsored Program Capacity Building Activities

1. CAREER preparation workshop
2. CAREER panels meeting to receive their comments
3. Nghia Chiem, Licensing Associate, University of Tennessee Research Foundation
4. SimCenter Energy Thrust at UTC
5. Jeffrey B Cornett, Manager, Industrial Partnerships & Economic Development at ORNL
6. Kashif Nawaz, Senior Research Scientist at ORNL

WHAT'S NEXT FOR THIS RESEARCH?

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

With preliminary data and modeling results mentioned above, 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.

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 solar energy harvesting and energy efficient building applications. The PI received another CEACSE grand utilizing aerogel for this year. Please, note that aerogel can enhance the water harvesting efficiency by increase the swing temperature for vapor desorption from the water harvesting device. The PI will focus on both water harvesting and solar energy conversion for the upcoming years.

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 one PhD student for the upcoming year hoping that improves research power. In addition, the PI plan to hire more undergraduate researchers via CEACSE fund and URaCE URTOPS Program.

FINANCIAL ACCOUNTING

During the unexpected Spring semester in 2020, the PI was not able to hire undergraduate researchers because of COVID-19. As a result, $1,408 is remined and is carried-over for the use of the following semester.

CEACSE Program – Final Report on Research Results

The Tasks and Timeline with Milestones/Deliverables

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

Description \ Month	1	2	3	4	5	6	7	8	9	10	11	12
Fabrication of 3dCN/zeolite adsorption layers												
Synthesis of 3dCN												
Fabrication of 3dCN/zeolite composite												
Computational device design optimization												
Develop 1D model for heat/mass transport												
Experimental characterization												
Validate the model results from labtesting												
Devices testing with a dynamic ads. System												
Builing a dynamic ads/des chamber system												
Testing fabricated adsorption layers												

Research Results

1. Synthesis and characterize the novel 3dCN

This project proposes the use of a novel melamine-derived graphene foam for use in a water harvester to replace previously used copper foam. Carbon foams have a documented ability to store thermal energy, and are flexible and lightweight, properties which are necessary for the development of a water harvester.[1] This project uses a novel graphene foam designed by Chen et al., which uses a high temperature pyrolysis to generate a high-quality graphene foam, using melamine foam as a source material. This foam has shown to be lightweight, flexible, and highly thermally conductive. Therefore, it has the potential to be an effective thermal conductor for use in water harvesting technology, while providing a solution to the problems associated with the use of MOFs. It should be noted that graphene foams, such as the one synthesized by Chen et al., are hydrophobic. In fact, they have proven to be effective in oil absorption. Despite the potential advantages of using carbon foam, infiltration of hydrophobic carbon foam with adsorptive crystals can be challenging due to the weak surface interaction between carbon foam and adsorptive crystals. Though this material has not previously been used for water harvesting purposes, the infiltration of hydrophobic carbon foam which absorbents has previously been performed by functionalizing the foam surface with strong acids and then saturated with a 50% zeolite solution.[2] Therefore, the use of graphene foam saturated with an absorbent has the great potential for use as an absorbent unit to enhance gravimetric and volumetric water harvesting efficiency. This project entails the synthesis and characterization of such a material.

The goal of this portion of the project will be to optimize the ramping rate, annealing temperature, and annealing time in order to yield a product of the highest purity possible. 1 cm cubes of melamine foam

were prepared and heated under inert conditions heated at a ramping rate of 5 °C per minute until final annealing temperatures of 700 °C to 1000 °C. In order to ensure that results were not skewed from allowing the more time to for the apparatus to reach the higher temperatures, the annealing time was manipulated so that the total reaction time was a constant 250 minutes. SEM images were taken of each sample as shown in Figure 1 and 2. From Figure 1, it is evident that for the foam synthesized at an annealing temperature of 700 °C, each strand is coated with deformities. These are likely indicative of the sample being of lower purity than the other samples.

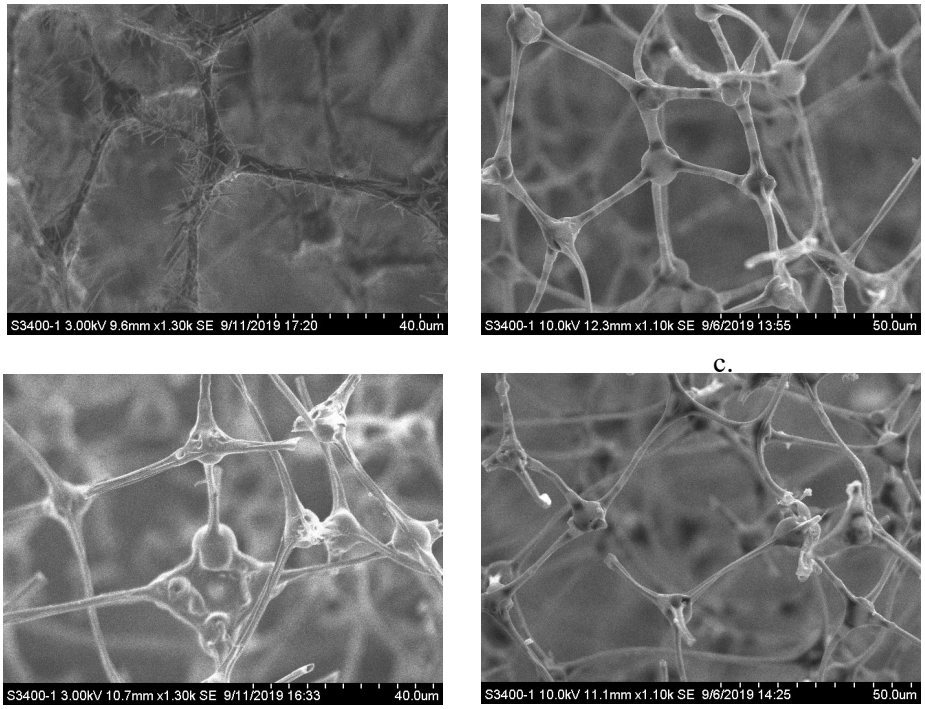


Figure 1: Low magnification: graphene foam synthesized at a.) 700 °C b.) 800 °C c.) 900 °C d.) 1000 °C

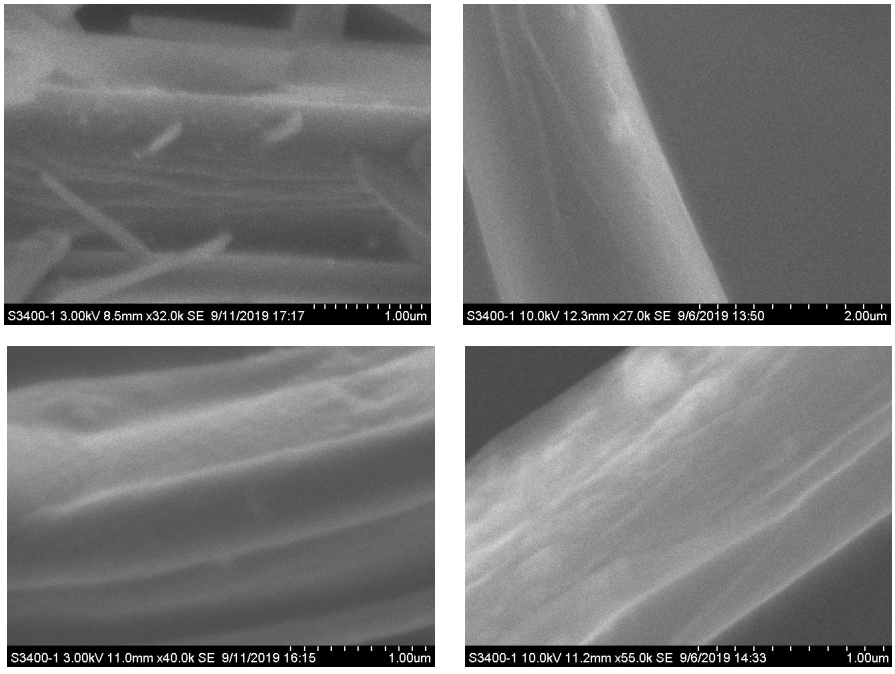


Figure 2: Low magnification: graphene foam synthesized at a.) 700 °C b.) 800 °C c.) 900 °C d.) 1000 °C

In addition, it appears from this set of images that the strands decrease in diameter as the annealing temperature increases. This may suggest that the purity is increasing as well, as noted by the change in structure. This change in diameter can be seen more clearly in Figure 2, where the diameter can be determined to vary from over 2 μm at lower annealing temperatures to roughly 1.5 μm at an annealing temperature of 1000 °C. The chemical makeup of these sample can be confirmed with Raman spectroscopy. Currently, these results are consistent with existing literature.

The quality (defects sites) of the synthesized graphene foam is analyzed using Raman spectroscopy. Graphite band (G band, ~1580 cm^{-1}) and disorder band (D band, ~1350 cm^{-1}) are correspoding to sp^2 carbon and sp^3 carbon. The higher G band, the higher quality graphite (less defects). On the other hand, the hgiher D band, the more defects on graphite. As shown in Figure 3, the higher annealing temperature, the more distinctive G-band indicating less defects on 3DGR samples. In addition, ramping rates of the annealing process will be tested. The ramping rate that yields the lowest defect sites will be used for the remainder of this project, in conjunction with the annealing temperature that yields the lowest defect sites.

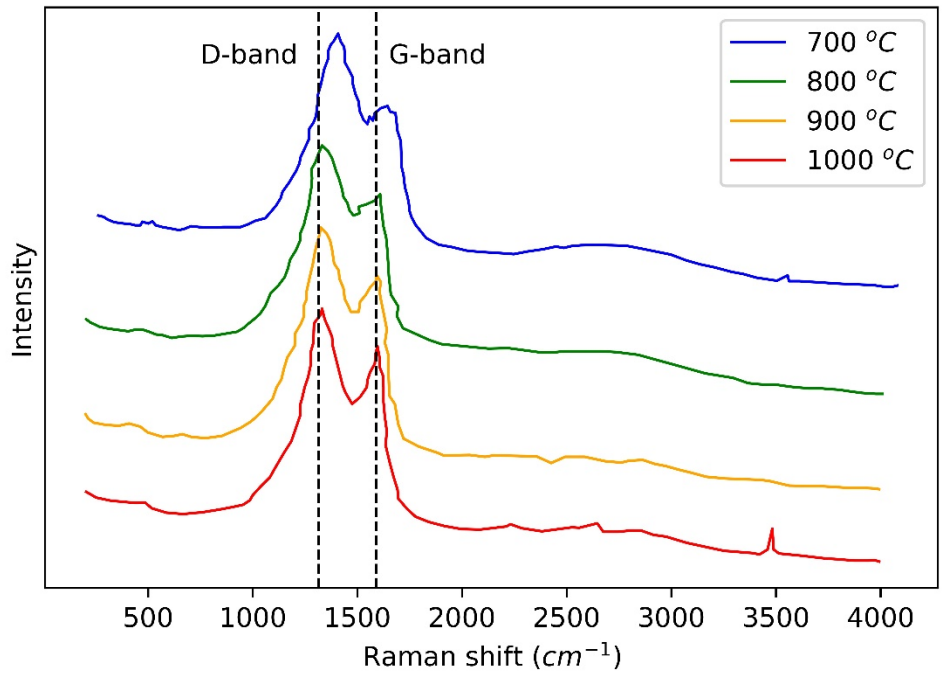


Figure 3: Low magnification: graphene foam synthesized at a.) 700 °C b.) 800 °C c.) 900 °C d.) 1000 °C

Due to the COVID-19, there have been unexpected delays on materials characterizations for 3dCN. However, for the following years, flexibility of the foam produced will be tested using compression testing and scanning electron microscopy (SEM). Compression testing will determine the overall elasticity of the foam following an applied stress. SEM will be used to compare the pore size and

deformation of the carbon foam before and after compression. In addition, the thickness and grain size of graphene within the carbon foam will be characterized by transmitting electron microscope (TEM). Following the optimization of the graphene foam procedure, this project will focus on addition of absorbent materials, in this case zeolite by functionalizing the surface of the carbon foam and using a hydraulic press, elasticity testing, further SEM imaging, imaging using a transmitting electron microscope (TEM), and vapor absorption testing.

2. Building a novel dynamic adsorption system

Without students researchers due to the COVID-19, building the dynamic adsorption system has been also delayed and still in progress. As shown in Figure 4, a water vapor resorvoir was installed to provide water vapor for the water havesting testing device inside of the chamber. Heating tapes was applied to provide heat for degasing. In addition, a solar simulator is added to mimic solar irradiation, which leads to water vapor desorption from adsorbents. A vacuum compatible gravimetry balance is in progress. Once we complete the dynamic adsorption system, we will perform detailed experiments to characterize and enhance the vapor diffusion characteristics (inter-/intra-crystalline diffusion) in device-level samples which dictate water harvesting rates. We will also perform systematic optimizations of the overall system architecture by leveraging our expertise in the development of high-fidelity adsorption computational models, which link molecular transport to system level characteristics such as water production (L kg-1 day-1) for a given heat input.

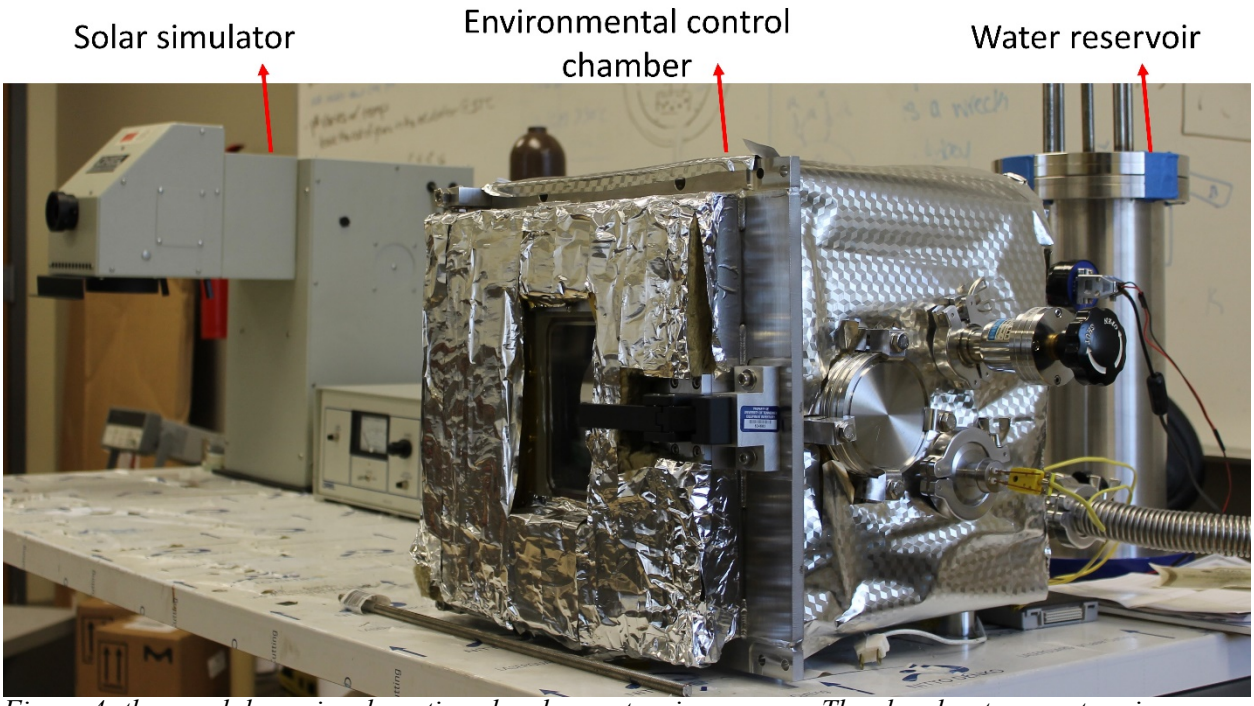


Figure 4: the novel dynamic adsorption chamber system in progress. The chamber temperature is controlled with a heating cable and variac power supply. A data acquisition system can be used to measure the adsorption layer, vapor, and condenser temperatures, and the heat flux readings. A power supply can be used to control the condenser temperature.

3. Building computational heat and mass transfer model

3.1 Modeling Project Objectives

The PI founded a Nanofluidics Chemical Engineering lab at UTC and began designing and acquiring specialized ovens, reaction chambers, instrumentation, and other equipment for the discovery and development of novel nano/micro porous structures. The computational group was established to assist in the design of novel structures and predict their characteristics. Computational work has been focused on the development of an adsorption based Atmospheric Water Harvester but the tools are intended to benefit several other projects being investigated.

Published computational work for adsorption based Atmospheric Water Harvesting, thus far, has been accomplished in modelers that solve on unknown mathematical assumptions. Those models require after the fact tinkering to bring the computed results in line with the experimental results. A principal objective of our efforts has been developing a Finite Element model that can explore nanomaterials using Darcy Navier Stokes equations fully characterized and solved with consideration to the mathematical assumptions typically hidden. Figure 5 shows the material properties and component-level properties we are investigating in adsorption based Atmospheric Water Harvesting. Our approach includes work towards optimization using topological techniques.

A secondary objective is to find modeling techniques for describing anomalous fluid behavior at the nanoscale. Of particular interest to the engineering of an adsorption based Atmospheric Water Harvest are condensation effects, fluid transport effects, and vaporization effects. Figure 6 illustrates behavior that can be studied using molecular dynamic modeling. Understanding the potential of an atmospheric water harvester optimized for anomalous behavior requires the study of such structures using molecular dynamics, an FEM model that is predictive and topologically shaped for heat/vapor transport.

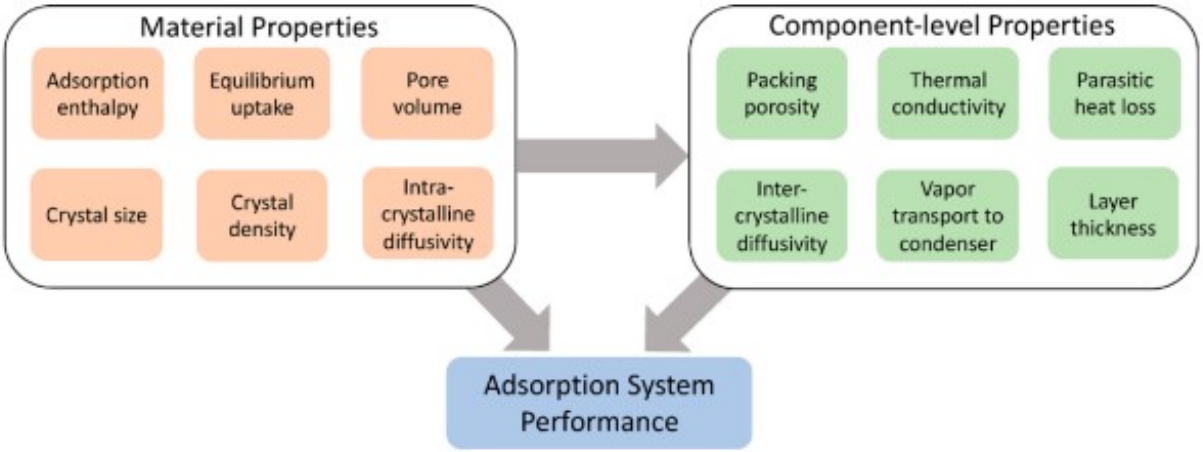


Figure 5: Finite Element Modeling, properties under investigation for optimization.

Over the course of this past year work progressed in the FEM modeling with comparison to benchmarks, FEM modeling with topological optimization, and molecular dynamic modeling. The work was completed in python. The FEM model was written in FEniCS and the molecular dynamics modeler was written in LAMMPS which is Python extensible. The work is being completed with consideration for tying together the FEM solver and the molecular dynamics model with optimization algorithms. Figure 8a

and Figure 8b show code generated meshes that can study device component dimensions under variable environmental conditions iteratively optimizing for vapor capture.

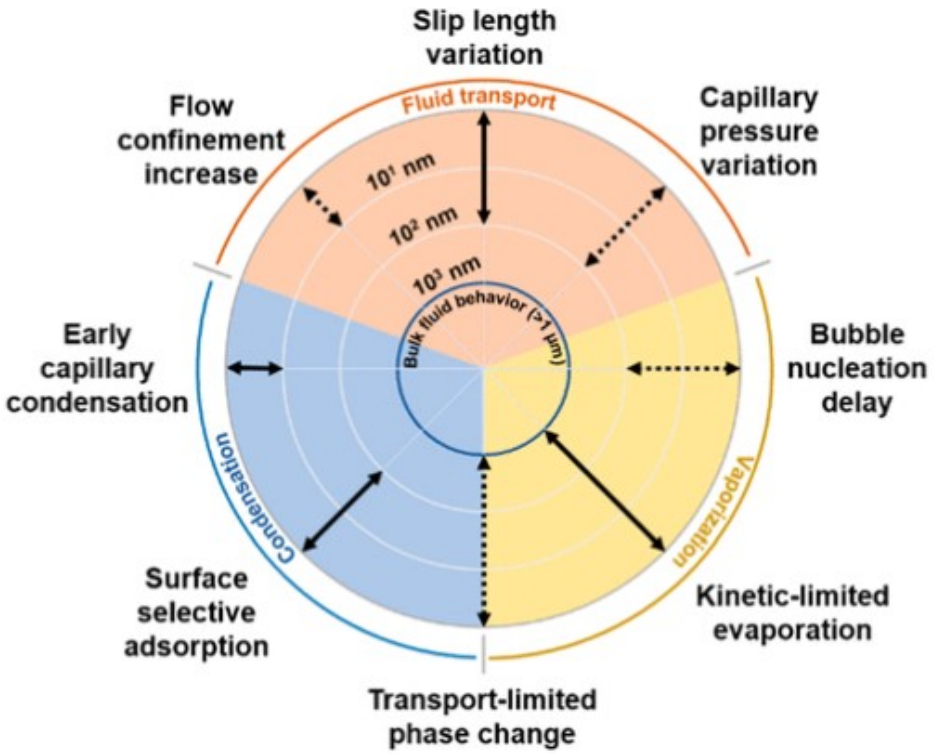


Figure 6: Key anomalies of nanoscale fluid behaviors. The double-sided arrows indicate the dimensions of interest for different anomalies and whether they promote (solid) or impede (dashed) fluid behaviors compared with classical bulk fluid theories.

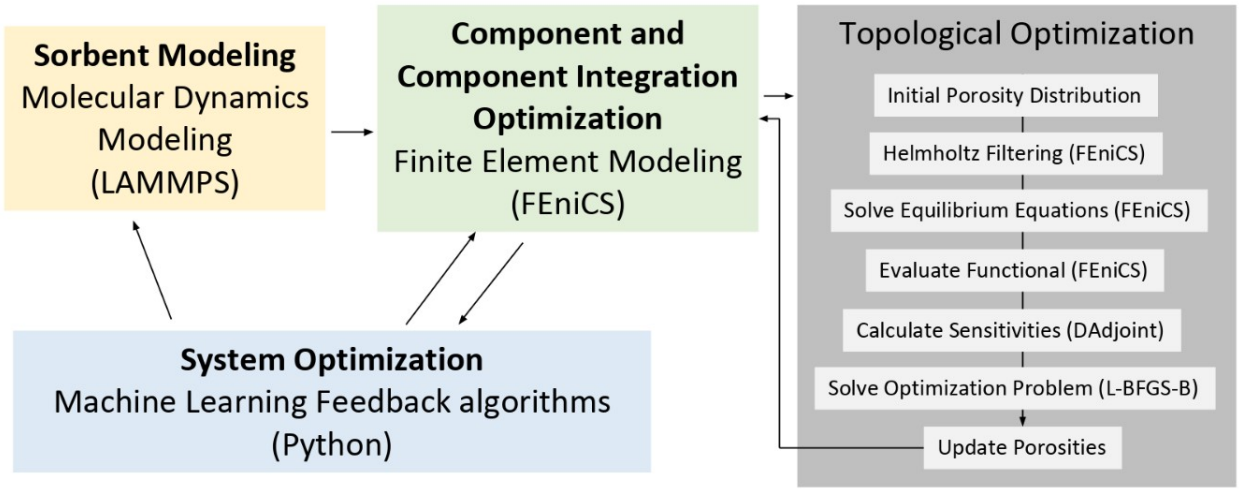


Figure 7: Potential code design for computational investigation.

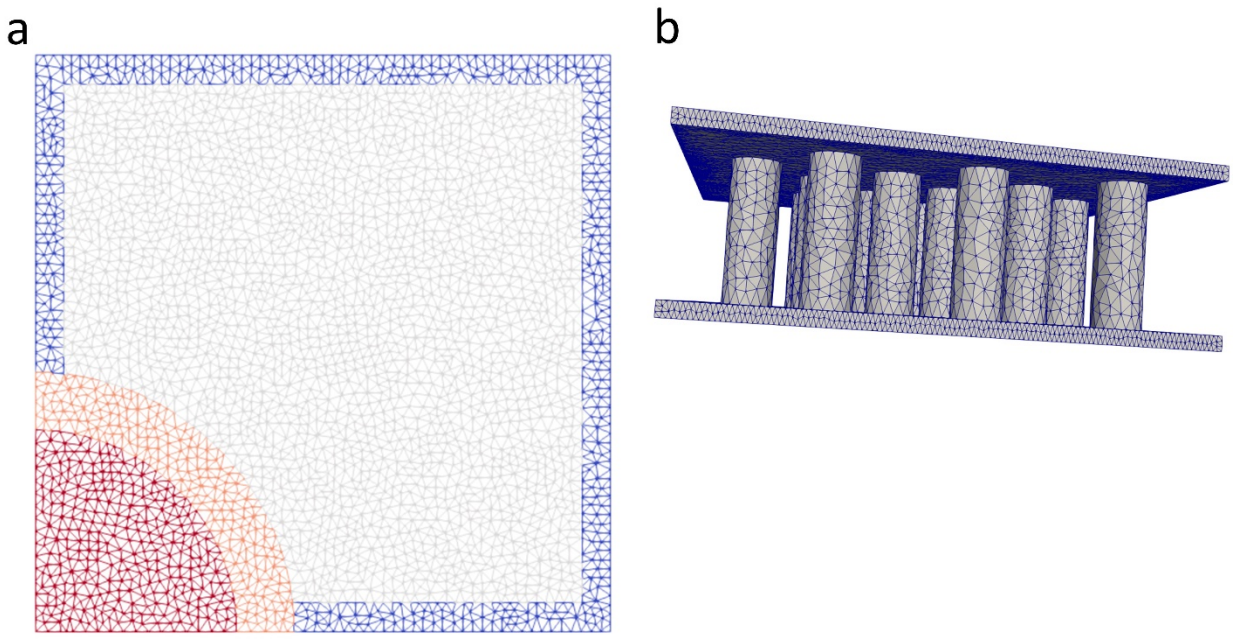


Figure 8: a. 2D mesh design with sub-domains - The orange represents sorbent for vapor capture, the blue represents a walled area, the red a sorbent or air gap for vapor release and collection, the grey represents open air flow. Mesh generated by code can be automatically adjusted by optimization algorithms. b. 3d mesh design - Two Copper heat sink/sources bookending sorbent rods. Rod diameter, length and copper thickness could be incorporated in an algorithm to increase adsorption/desorption cycling for vapor flux.

3.2 Finite Element Method modeling

3.2.1 Coupled Mixed Solver Dimmensionalized by Rayleigh

The first completed model solves a vapor flow system that is a steady-state Poisson equation with a thermal/concentration serving as a source term. The polynomial degrees of the shape functions were chosen to satisfy the inf-sup conditions. The Brezzi-Douglas-Marini (BDM) function space was chosen for velocity and a lower order discontinuous Galerkin (DG) function space for pressure, both are built on triangular element shapes. This element pair is frequently paired for solving the Poisson equation and hopefully ensures vapor continuity on elements. This also allows the velocity field to be interpolated continuously. The weak form of the thermal diffusion equation needs further development. There are a vast array of stabilization techniques if necessary. The diffusive term is currently being derived with the symmetric interior penalty (SIPG) method. A backward euler formula is used to discretize heat in time. The step size is updated according to the Courant-Friedrich-Lewy (CFL) condition. There are higher-order adaptive time-stepping methods to be evaluated. This numerical construction is producing results. It was necessary to evaluate computational cost, step size, and numerical error. The code used manufactured solutions fields in a unit square for pressure (p) = sin(x)cos(t) + cos(z)cos(t), velocity (u) = [-cos(x)cos(t),sin(z)cos(t)] and temperature (T) = sin(x)cos(t) + sin(z)cos(t), with Dirichlet boundary conditions. Tables 1 and 2 describe the Numerical Errors with respect to different choices of mesh size across its trial functions of Pressure, Temperature, and Velocity. The error calculations are an L2 of the

analytical solution and the computed solution. The order of error for pressure is 1 and the order of error for velocity and temperature fields is 2. The convergence rates should reflect that relationship. The computational cost in seconds per timestep have also been calculated. The convergence rates for velocity and temperatures cause me concern. I would expect them to be closer to 2. I will investigate code for improvements.

DG0-BDM1-DG1								
h	error(p)	rate(p)	error(u)	rate(u)	error(T)	rate(T)	DOF	cost
1/4	2.60E-02	0.00	3.16E-02	0.00	3.74E-02	0.00	240	4.32E-02
1/8	1.27E-02	1.03	1.11E-02	1.51	1.37E-02	1.45	928	1.71E-02
1/16	6.29E-03	1.02	4.36E-03	1.34	5.50E-03	1.31	3648	1.02E-01
1/32	3.13E-03	1.01	1.97E-03	1.15	2.51E-03	1.13	14464	1.28E+00
DG1-BDM2-DG2								
h	error(p)	rate(p)	error(u)	rate(u)	error(T)	rate(T)	DOF	cost
1/4	1.37E-03	0.00	1.12E-03	0.00	7.55E-04	0.00	552	6.65E-02
1/8	3.46E-04	1.99	2.55E-04	2.14	1.51E-04	2.33	2160	5.11E-02
1/16	8.69E-05	1.99	6.12E-05	2.06	3.43E-05	2.13	8544	3.60E-01
1/32	2.18E-05	2.00	1.50E-05	2.03	8.30E-06	2.05	33984	4.97E+00

Table 1: Convergence testing.

3.2.2 Horton Rogers Lapwood

A saturated porous medium with impermeable boundaries in a unit square box sets the stage for the first benchmark problem. The initial conditions are uniform in temperature and fluid flow with both at 0. The top boundary face is held constant at 0 the bottom face is uniformly heated to 1.
The average Nusselt number, Nu will be computed to describe the system as it evolves. The Nusselt number is the ratio of total convective heat transfer / conductive heat transfer. This benchmark will allow us to consider a given Rayleigh number and the resulting Nusselt number. The simulations will begin with a Rayleigh number slightly below the critical Rayleigh number, which is the value below which heat is transferred purely by conduction. Each Rayleigh number will be run into the resulting Nusselt number is at steady-state. The solution is saved and used as initial conditions for the next stage. The symmetric initial condition of the temperature field could cause a loss of solution uniqueness. A small sinusoidal perturbation was made on the temperature field on the bottom face boundary. Figure 9a and Figure 9b show the expected initial and resulting Temperature/Velocity Flow plots for the Horton-Rogers-Lapwood benchmark. The resulting Nusselt numbers do not match reference Nusselt numbers from (Schubert and Straus 79).

Ra	32 x 32	48 x 48	64 x 64	Reference
100	1.016257	1.007266	1.016225	2.651
150	1.007266	1.003247	1.007237	3.322
200	1.004111	1.001837	1.004089	3.808
300	5.104870	4.548784	4.544925	4.510

Table 2: Mesh size was varied to find agreement with output Nusselt to reference. Agreement did not begin until Ra 300. The model can be improved and this will be further investigated. The benchmark allows us the ability to verify accuracy.

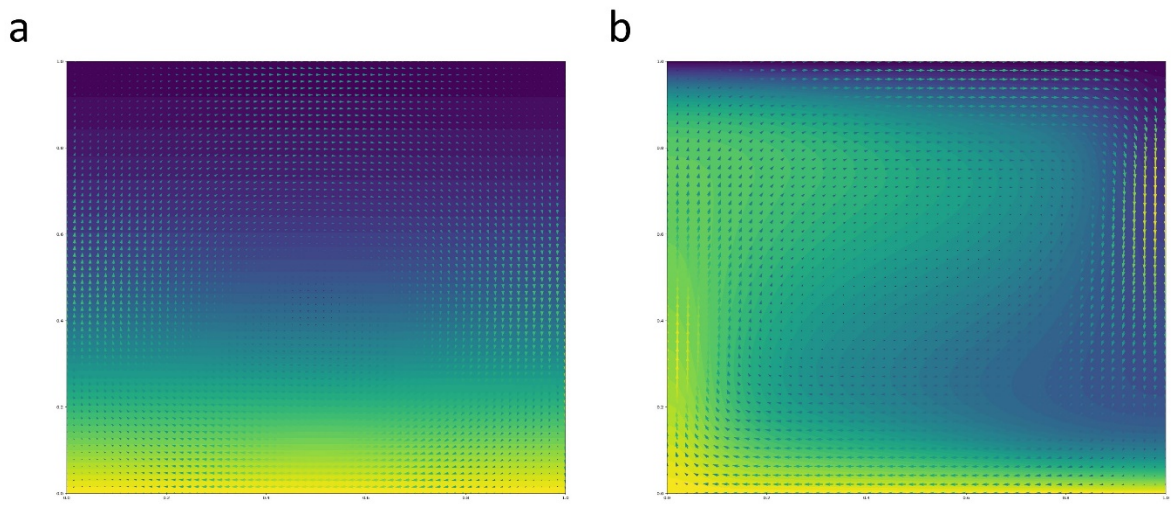


Figure 9: a. Horton-Rogers-Lapwood at timestep 1. The heating from the bottom plate is poltted with the yellow. The arrow glyphs describe fluid velocity vectors. The visualization represents what would be expected from this model. b. The Horton-Rogers-Lapwood reached steady state with Rayleigh Number 300. A clockwise motion has emerged in the fluid flow. This was the Ra number in agreement with reference. The rotating motion was the desired visualization resulting from the boundary conditions and indicates solver confidence.

3.2.3 Heating from Right Side

Like the Horton-Rogers-Lapwood problem, the heating from side is a unit square box of porous medium represented in the Figure 8 and 9. One side boundary face is held at T =1 and the other side boundary face is held at T=0 for the duration of the simulation, with the domain initially at T=0.
The side to side temperature differentials conduct heat across with buoyancy effects first driving fluid upwards near the warm wall and continuing in a circular motion. The Nusselt number can be used to measure heat transfer. driving the fluid near the left boundary which then The heating from the side problem has a unique solution. The same solver was used in heating from the side as for Horton-Rogers-Lapwood except for a CFL adjustment to keep the solver from crashing. Restoring the CFL and adjusting the timestep should bring the HRL solver into agreement with references.

Ra	32 x 32	48 x 48	64 x 64	Reference
100	3.135038	3.117636	3.113049	3.103

Table 3: Mesh size was varied to find agreement with output Nusselt to reference. Agreement with the found reference of 100 was good.

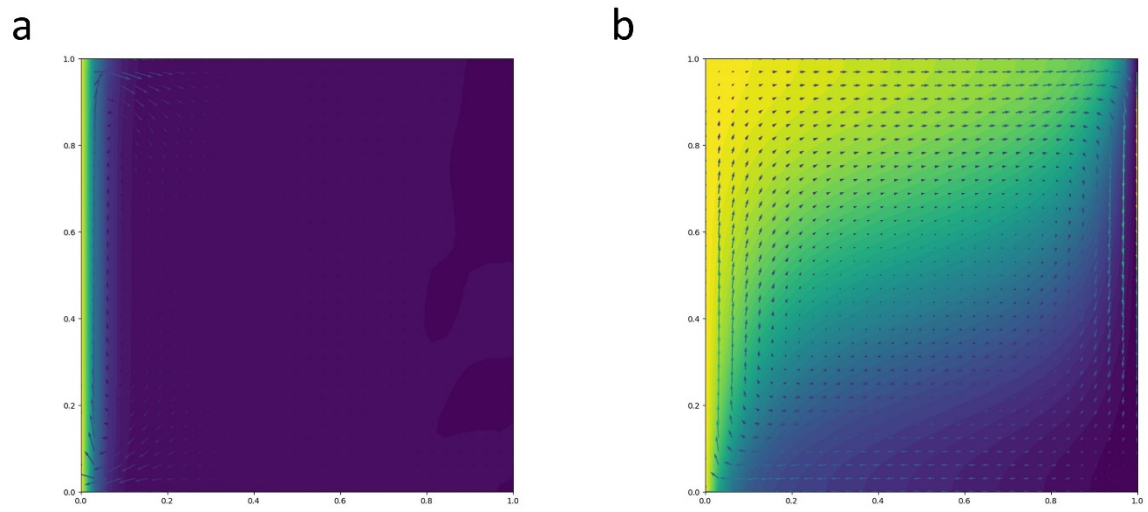


Figure 10: a. Heating from the side at 1st timestep. Visualization properly describes setup. b. Heating From Side - Steady State reached at Rayleigh Number 130. Buoyancy effects of heat are dominating fluid flow with similar circular pattern forming as Horton-Lapwood-Rogers.

3.2.4 Usage

The first FEM solver successfully solved two benchmarks. The benchmarks can be used to evaluate solver accuracy and for consideration of materials under investigation. The development of the first model allowed a stepping stone for development of more sophisticated models. The first model will be of tremendous use in investigating buoyancy driven heat flows.

3.3 FEM modeling with Topological Optimization

The goal of topological optimization is to modify the shape and connectedness of a domain so that a objective function is minimized. Shape optimization is limited to adjustment of boundaries. Topological optimization can be used to adjust features in a domain. In 2003 Borvall and Petersson applied topological optimization on the stationary Stokes flow. Before this shape optimization was principally used. Guest and Prevost extended work on a relaxed Stokes flow formulation where the impermeability worked as a penalty factor on the flow velocity, by applying a stabilized finite element formulation for the Stokes Darcy equations treating the solid phase as a porous medium. Gersbrg-Hansen implemented a topological optimization for Navier-Stokes equation in 2005 with a proposed analytical sensitivity analysis using adjoint. In 2018 Ricardo Amigo described a topological optimization method applied to a gas adsorption system utilizing highly porous material's. Our goal is to implement Amigo's scheme which is described in Figure 7. Work has proceeded with proper execution of a Naiver-Stokes-Darcy scheme with PDE-constrained optimization and sensitivity analysis. A new Finite Element Variational Formula for our nanofluidic system is being written. It is forward looking equation and will be fully specified with thermodynamic characteristics. A material model based on offset hyperbolic tangents is suitable for this kind of optimization. Checkerboard instability and mesh dependency are filtered by smoothing Helmholtz-type PDE, based on a implementation goals for our TOM.

3.4 Molecular Dynamics Modeling

The kinetics of adsorption consists of three steps (i) mass transfer of the adsorbate from the solution to the external surface of the adsorbent, (ii) diffusion through the adsorbent and (iii) adsorption itself. When modelling adsorption kinetics it is usual to assume that either the diffusion or the actual adsorption is the rate limiting step and dictates the rate of the process as a whole. A key issue is determining which assumptions are correct. Two main models are reported for adsorption kinetics taking the intra-particle diffusion as the rate limiting step: Crank and Weber-Morris. Crank assumes homogenous diffusion across an adsorbate consisting of spheres. The Weber-Morris uses an empirical observation that varies nearly proportionally with (t).5 and an empirically intra-particle diffusion rate. When the adsorption itself is the rate limiting step, Elovich or Lagergren equations are used to model q. Elovich uses an empirically discovered variation in its formula. Lagergren models are in fact a family of models, many of which rely on empirically derived constants.
The reliance on empirically driven models is a bottleneck in determination of adsorbant capability. Currently we can only be surprised in the lab. The two main goals for a molecular dynamics model is to verify we can accurately model material thermodynamic properties from computational work and to better understand the physics of adsorption/desorption. There is potential to publish in both areas. Figure 11c is a simulation of water molecules proceeding through carbon nanotubes. The rapid transport of water and the conduction of adsorption generated heat are of critical importance in maximizing water harvesting potential. Studying the formation of Zeolites can help in the understanding if its possible to develop complicated Graphene Zeolite hybrids.

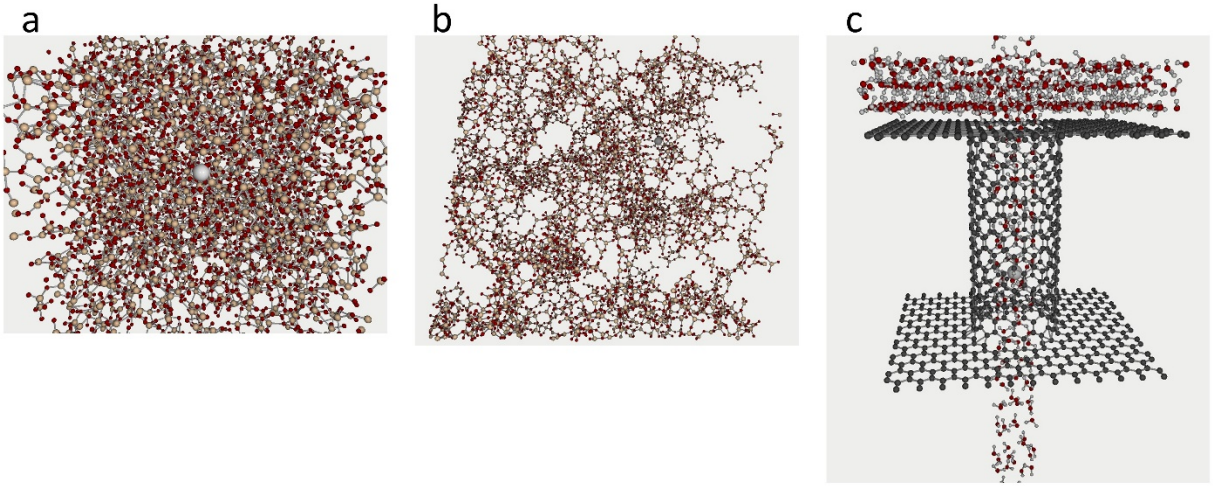


Figure 11: a. Simulation of the formation of Nanoporous silica using Vashista potential. This figure shows the underlying materials before structure formation. b. The zeolite at timestep 8000 has formed with intracyrstal porosity's visible. LAMMPS can compute thermal conductivity's and water vapor transport velocities. c. Water through a carbon nanotube using the Vashista potential

3.5 Computational modeling conclusion

Work has progressed on several codes and techniques for engineering nanofluidic materials. The goals for the next year are to bring these threads together. The areas are not well-established fields of computational research and require continual questioning of assumptions and theory.

Expected Outcomes and Updates

The success of this project will be based on achievement of the outcomes outlined above, namely:

1. Successful collection of relevant data for water harvester by 2020 Summer
   - Delayed by COVID-19. However, the PI plans to continue the proposed research in the following semesters.
2. Poster presentation of the results by the undergraduate students at ACS or MRS meeting in 2020
   - Delayed by COVID-19.
3. Proposal submission for CRISP, internal grants at UTC by 2020 Fall
   - Since CRISP was no longer available, the PI applied another CEACSE grant and won it.
4. Three publications of the results in peer-reviewed journals between 2020 and 2021 Fall
   a. **Publication 1**: Thermal and Mechanical Properties of 3-Dimensional Carbon Network (3dCN) as Flexible Thermal Additives
      - In progress. The PI plan to continue working on 3dCN to get a peer-reviewed publication. (~50% completed)
   b. **Publication 2**: Optimization of The Adsorbent Geometries of Water Harvesting System by Finite Element Method
      - In progress. The PI plan to continue working on FEM modeling to get multiple peer-reviewed publications. (~70% completed)
   c. **Publication 3**: Simultaneously Enhanced Heat and Mass Transfers Using Flexible Carbon Foam for Highly Efficient Water Harvesting Systems
      - Delayed. Due to COVID-19, lack of student researchers over Spring semester and the summer in 2020.
5. Submission of an ONR grant by Summer 2021 with Dr. Antao
   - In progress.
6. Submission of a NSF CAREER grant by Summer 2022
   - In progress.

Plan to Extend and Sustain Research/Scholarly Activity / External Funding

With preliminary data and modeling results mentioned above, 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.

RERERENCE

(1) Chen, Z.; Ren, W.; Gao, L.; Liu, B.; Pei, S.; Cheng, H.-M. Three-Dimensional Flexible and Conductive Interconnected Graphene Networks Grown by Chemical Vapour Deposition. *Nat. Mater.* **2011**, *10* (6), 424–428. https://doi.org/10.1038/nmat3001.

(2) Yang, S.; Huang, X.; Chen, G.; Wang, E. N. Three-Dimensional Graphene Enhanced Heat Conduction of Porous Crystals. *J. Porous Mater.* **2016**, *23* (6), 1647–1652. https://doi.org/10.1007/s10934-016-0225-9.

Fiscal Year 2020 Final Project Report
Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Fernando Alda-Pons, Lead PI

Other Personnel: N/A
Project Title: "Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)"
Date Report Submitted:
Award Start – End Date: August 1, 2019 – May 31, 2020
Non-Technical Summary:

There are more fish species in the world than among all the other vertebrates combined. About half of all fish species are confined into rivers and lakes, most of which occur in the Neotropics. The enormous diversity found in the Neotropical region makes it an ideal scenario to explore the processes and mechanisms that have originated such outstanding diversity and furthermore, to understand how species originate. In this project, I used massive parallel sequencing technologies to reveal the molecular and genomic basis of the speciation process using a group of Neotropical electric fishes as a study system. I compared the patterns of evolution among genes that are involved in the generation of electric signals and genes that are expected to evolve under a neutral process and developed a model for the evolution of this communication mechanism. Based on this model I hypothesize that the origin of this behavior is more complex that originally proposed and that has appeared multiple times in this group of fishes facilitating the origination of new species.

The activities that I carried out included a trip to Colombia in the summer of 2019, during which I collected samples of electric fishes and instructed a course on phylogenomic methods. I recruited two UTC undergraduate students that worked during the 2019-2020 academic year and will continue their research in my lab this upcoming year. One of my students benefitted from a grant from the Honors School and will make this project part of her Departmental Honors Thesis. She submitted her work to UTC's Research Dialogues undergraduate symposium. My other student was accepted in UTC's iCompBio REU program organized in collaboration with the SimCenter, during which she is developing computational tools that will be applied to the data obtained from this project. Also, I participated in outreach activities like the science café Chatt About Science. This project has allowed interaction and new collaborations with other faculty associated to the SimCenter that are resulting in new proposals that expand on this project and also aim to develop novel research lines.

PROJECT TITLE: Models of speciation based on the evolution of electric communication in weakly electric fishes (Gymnotiformes)
Technology Area of Interest: **Health and Biological System**

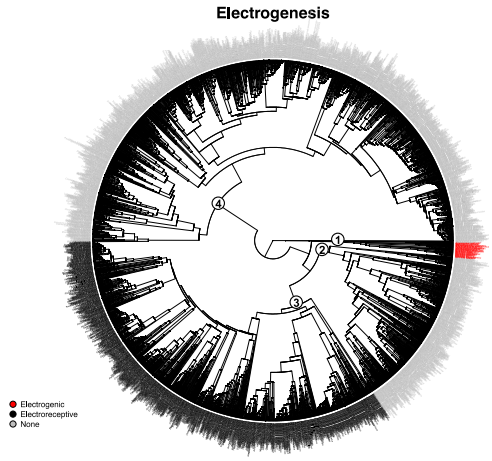
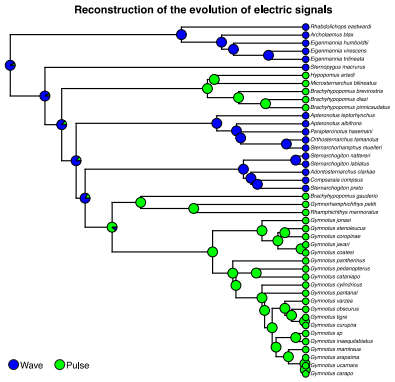
TECHNICAL APPROACH	OUTCOMES
I proposed to compare genomes and transcriptomes of tissues involved in the generation and interpretation of electric signals among and within species, to determine the relative roles of neutral and selective forces in generating this diversity. The main aim is to identify mechanisms and evolutionary forces involved in diversification of electric communication, and to assess its role as a motor of speciation. *Tasks* 1. Collection of samples 2. Genomic data analysis 3. Comparison of adaptive and neutral genes 4. Construction of evolutionary model of speciation 5. Identification of orthologs and differential gene expression	We have collected tissues for RNA sequencing and differential gene expression analysis from 8 species of gymnotiforms and collected fish from 5 localities in the wild in Colombia. We have obtained genomic data for 44 species of gymnotiform fish species. The main outcomes of this project have been submitted to UTC's Research Dialogues by undergraduate student Tiffany Harvey.
RESULTS	**OTHER INFO**
Fig.1  	*Budget and Schedule* Total Budget: $ 24,949 Actual Used: $ 24,575 Balance: $ 373.79 Total period of performance is 12 months. Task 1: Months 1-2 Task 2: Months 3-8 Task 3: Months 8-11 Task 4: Months 10-12 Task 5: Months 11-? *Deliverables*

Fig.2



- Monthly report describing numerical methods, techniques, and results that were developed or improved.
- 3/9/2020 mini-CEACSE Midterm Report
- 30/6/202 mini-CEACSE Final Report
- Final report detailing results, financials, and future work

Publications

- Harvey T, Alda F (2020) Revised phylogenetic hypothesis and comparative evolution of mitochondrial genomes of Neotropical weakly electric fishes (Gymnotiformes). *ReSEARCH Dialogues Conference Proceedings.*

External and internal conference presentation

- 2020 UTC Research Dialogues ReSEARCH Dialogues Conference Proceedings.
- 2020 Joint Meeting of Ichthyologists and Herpetologists, Richmond VA. Cancelled due to COVID-19.

Organization Information

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ACCOMPLISHMENTS & OUTCOMES

Project Overview

I hypothesize that the evolution of electric communication has played a major role in the process of speciation of gymnotiform fishes. Therefore, I expect to see larger differences in the rate of evolution and gene expression in genes involved in the generation, reception and processing of electric signals than in genes not involved in these mechanisms. I proposed to compare genomes and transcriptomes of tissues involved in the generation and interpretation of electric signals among and within species, to determine the relative roles of neutral and selective forces in generating this diversity. The combination of genomic and transcriptomic surveys at different taxonomic and geographical scales will allow me to identify mechanisms and evolutionary forces involved in diversification of electric communication, and to assess its role as a motor of speciation.

We have obtained genomic data for 44 species of gymnotiform fish species using massive parallel sequencing technologies. We assembled raw reads from pair-end Illumina sequencing machine into complete mitochondrial genomes. Undergraduate student Taya de Blonk has worked on an automated bioinformatic pipeline for assembling and annotating mitochondrial genomes using next generation sequencing data. Furthermore, Taya is participating in the iCompBio REU program by testing the efficiency of her pipeline and comparing it to other assemblers available.

We combined newly generated genomic data together with available complete genomes from 3353 taxa of the superorder Ostariophysi to reconstruct the evolutionary relationships and origin of electrogenesis (Figure 1). We used a maximum likelihood inference method of the concatenated data, as well as for each gene separately. We compared rates and patterns of DNA substitution between genes that are involved in the production of energy in electric organs and genes that carry cell housekeeping functions or non-coding (Harvey and Alda, 2020). We expect that those genes involved in electric signal generation are under stronger selective pressures and show larger base compositional bases compared to genes that do not deviate from the expected neutral model of evolution. Within the electrogenic order Gymnotiformes, we used 500 simulations of stochastic character mapping using the R package phytools to reconstruct the evolution of their different electrocommunication systems and type of electric signals. Our evolutionary and speciation model supports multiple events for the origin of electric signals (Figure 2). Neither the families Apteronotidae and Sternopygidae nor Hypopomidae, Rhamphichthyidae and Gymnotidae that produce, respectively, wave-type and pulse-type electric discharges form reciprocally monophyletic groups. Our model, therefore, suggests a more complex mechanism than initially proposed for the development of electric organs and their role in speciation. Our main results have been submitted to UTC’s Research Dialogues by undergraduate student Tiffany Harvey.

We have also collected and submitted tissues for RNA sequencing and differential gene expression analysis from 8 species and from 5 localities for one of them, which are used for comparison at different taxonomical and evolutionary scales. These samples are

being sequenced by Novogene (see below). This work is part of the research carried out in my lab by student Taya de Blonk.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Collection of samples	Accomplished
Genomic data analysis	Accomplished
Comparison of adaptive and neutral genes	Accomplished
Construction of evolutionary model of speciation	Accomplished
Identification of orthologs and differential gene expression	Unfinished

Challenges & Strategies Used to Address / Overcome:

In my original proposal, I considered the possibility of short-term maintenance of fish in the animal facilities at The University of Tennessee at Chattanooga. I requested IACUC approval to carry out the activities proposed activities but to this day, these facilities are still non-functional. Because of this delay, I had to change the plan and methodology of the project.

Regardless, I have collected wild specimens of Glass knifefish of the genus *Eigenmannia* from two Colombian drainages (Orinoco and Magdalena) and five species from four families of electric fish from commercial suppliers: *Apteronotus rostratus,* Black ghost knifefish; *Apteronotus albifrons,* Brown ghost knifefish; *Eigenmannia virescens,* Glass knifefish; *Steatogenys duidae,* Centipede knifefish; *Brachyhypopomus gauderio,* Bluntnose knifefish. From all specimens, I have obtained four types of tissues Electric organ, brain and muscle for RNA analysis and an additional muscle sample for DNA analysis. Total RNA will be extracted from these tissues are being sequenced and analyzed by Novogene: Genome Sequence Company. Samples of *Eigenmannia* will be used to compare within-species variation and the other specimens will be included in comparisons among species at a higher taxonomic level.

Covid-19 has also affected other activities proposed for this project. Following the cancelation of all face-to-face activities at UTC it was not possible for my student Taya de Blonk to access the laboratory to carry out the analysis and processing of the RNA samples. Furthermore, this work was going to be part of Taya's project during the iCompBio REU program. We were forced to change our plan into a purely computational project dealing with the development of a bioinformatic pipeline for the assembly, annotation and analysis of genomes. This task is still relevant and useful for the overall project proposed.

Also, the epidemic has delayed the analysis of RNA samples because sequencing companies are dedicated almost exclusively to the analysis of SARS-CoV-2 samples. This has increased their backlog and turnaround times. I expect that the sequencing of our samples will be finalized during fall 2020 so we will be able to complete the task #5 of the project.

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

Most of the challenges faced during this project were due to issues related to our department's building renovation and covid-19 (see above).

IMPACT & OUTCOMES

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

This project has allowed me obtaining new data that will be useful for developing stronger research hypotheses that will be used in future research applications. I have plans to travel again to Colombia and maybe to Brazil, depending on the travel situation in the following months, and hopefully these preliminary results will help me develop new projects and collaborations.

Also, have established new collaborations with other UTC faculty, particularly with Dr. Yu Liang from the Department of Computer Science and Engineering. We have already submitted an application for a non-related project that also involved the SimCenter.

Students Impacted

I have recruited two UTC undergraduate students to work in this project:

Taya de Blonk is a senior at UTC and will be graduating in the Fall of 2020. She has been working in the collection and dissection of tissues for RNA extraction and on the development of an automated bioinformatic pipeline for the assembly, annotation and analysis of genomic data. During the Summer of 2020 she is involved in the iCompBio REU program.

Tiffany Harvey is a transfer student from Chattanooga State. Tiffany has been working on the analysis of genomic data and the comparison of genes involved in the generation of electric signals. She was awarded a grant from the Honors School to work on her project during the Spring of 2020 and she will continue working on this project as part of her Departmental Honors Thesis during the academic year 2020-2021. Tiffany has also been a recipient of the Craig Scholarship awarded by the Department of Biology, Geology and Environmental Science for her research accomplishments during the past year.

Community and Broader Impacts

As a complement to the proposed project I was organizing the 2nd Edition of the Southeastern Computation School in collaboration with the SimCenter and BGE. The SimCenter was providing funding to bring instructors from Michigan State University and

cover expenses for students attending the course. This workshop was cancelled due to Covid-19

Scholarly Products

Publications:

Non-Refereed Conference Proceedings

- Harvey T, Alda F (2020) Revised phylogenetic hypothesis and comparative evolution of mitochondrial genomes of Neotropical weakly electric fishes (Gymnotiformes). *ReSEARCH Dialogues Conference Proceedings.*

External Conferences (Cancelled)

- I had submitted an abstract to present work related to this project at the 2020 Joint Meeting of Ichthyologists and Herpetologists but this conference was cancelled due to Covid-19.

Presentations at UTC:

- Harvey T, Alda F. 2020 Research Dialogues. Poster.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

Collaboration

I have established new collaborations with other UTC faculty, particularly with Dr. Yu Liang from the Department of Computer Science and Engineering. We have already submitted an application for a non-related project that also involved the SimCenter.

Outreach:

On 11/20/19 I participated as a speaker in the science café Chatt About Science. I gave a talk about the diversity and evolution of electric fishes entitled: *These fishes will shock you!*

EXTERNAL FUNDING

Proposal Submissions

One UT Collaboration Grant

Contracts/Awards Received

N/A

Sponsored Program Capacity Building Activities

- Attended the CAREER grant preparation workshop organized at UTC by T.I.G

- Met with Ashley Ledford, Grants Administrator from the College of Arts and Science to discuss funding opportunities.

WHAT'S NEXT FOR THIS RESEARCH?

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

Given the delays in the sequencing and analysis of the RNA samples that task of the project remains unfinished. I expect to receive sequencing data back from Novogene Sequencing Company during the Fall of 2020 so I could complete the analytical part of this project.

In the following year, my students Taya de Blonk and Tiffany Harvey will continue working in their respective subprojects. I expect that at least two manuscripts can result from this work.

I have plans to travel again to Colombia and maybe to Brazil, depending on the travel situation in the following months, and hopefully these preliminary results will help me develop new projects and collaborations. Based on these results and interactions I plan to write a proposal to be submitted to NSF during the summer of 2021.

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

My main research interests are related the diversity and evolution of Neotropical fishes, therefore, all of my work is directly and indirectly impacted by the support received from CEACSE. I expect to continue using these resources for my research with people within and outside of UTC.

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 2020 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Stephanie DeVries, Lead PI

Other Personnel: N/A

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

Date Report Submitted:

Award Start – End Date: August 1, 2019 – May 31, 2020

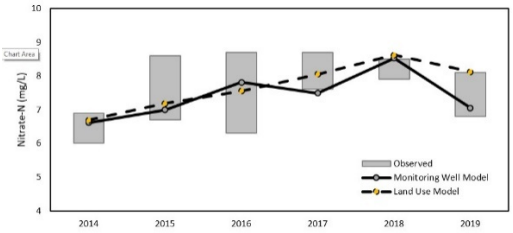
Non-Technical Summary:

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

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

PROJECT TITLE: A simplified subsurface characterization for local-scale groundwater flow models in unconfined sand and gravel quivers.
Thrust Area: Health & Biological Systems

PROPOSED TECHNICAL APPROACH	OUTCOMES
The following technical approach includes items from the original and modified proposal activities. • Develop a 3D geologic framework model of subsurface in Rockworks 3D. • Develop a geostatistical model of subsurface with SGeMS. • Run groundwater flow and particle transport simulations using MODFLOW and MODPATH codes and perform a statistical comparison of capture zones delineated by 3D geologic framework model, geostatistical model, and novel Thiessen Polygon model of subsurface. • Develop a spreadsheet model to estimate nitrate concentrations at a pumping well as a function of land use and travel time inside MODPATH-delineated capture zone. • Develop a Python model to perform the same calculations as the above-referenced spreadsheet. Calculations based on user-provided recharge, USDA CropScape data (ASCII), a lookup-table, and travel-time/capture zone (ASCII).	Only a small portion of the original proposal was completed as planned. A borehole database was constructed in Rockworks 3D and used to generate a 3D geologic model of the project area subsurface in Rockworks but technical difficulties prevented the next step, which involved “slicing” the 3D model for gridded input into the groundwater model. In the absence of a completed geologic framework dataset by March 2020, it did not make sense to continue work on that approach so efforts to prepare a geostatistical model in SGeMs and perform the groundwater flow comparison were suspended. As an alternative, a spreadsheet model was developed to estimate nitrate concentrations at a pumping well as a function of land use and travel-time inside a MODPATH-delineated capture zone. This model is pending review as part of a Technical report submitted to the Wisconsin Geologic and Natural History Survey. A Python-based version of this model was developed and coded to allow broader flexibility and use of this tool in applicable geologic environments.

RESULTS	OTHER INFO
• Spreadsheet model of mean annual nitrate concentration at municipal fit to observed data within 5% (see Figure below)  • Python model estimated nitrate concentration for 2019 at 8.68 mg/L vs. 8.43 mg/L calculated by spreadsheet, which is within the expected margin of error based on differences in the way area and recharge are entered into each model. A graphic of the model output in terms of mg NO3/grid cell is shown below. • 	**Budget and Schedule** Total Budget: $24,981.00 Actual Used: $20,707.28 Balance: $ 4,273.72 **Deliverables** • Spreadsheet Model submitted for publication as part of a Technical Report (Wisconsin Geologic and Natural History Survey). • Invited to present the model to Wisconsin DNR by Zoom conference. • Abstracts submitted to AGU and GSA to present model at fall 2020 conferences. **Deliverables** Department of Biology, Geology, and Environmental Science

ACCOMPLISHMENTS & OUTCOMES

Project Overview

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop a Geologic Framework Model for Waupaca, WI, well capture zone	Borehole database and 3D framework model successfully constructed. Conversion of model to input for groundwater flow model is incomplete/pending.
Develop a statistical model of subsurface for Waupaca, Wi, well capture zone	Incomplete/Pending
Run groundwater simulations to compare flowpaths and capture zone simulated using geologic framework model, stastical model, and theissen-polygon model.	Incomplete/Pending
Develop a spreadsheet-based model that estimates well nitrate concentration as a function of historical land use, annual recharge, and groundwater flow.	Model successfully created. Model predictions are within 5% of observed annual range of nitrate concentrations for two wells in years 2014-2019.
Convert spreadsheet-based nitrate model into a standalone python executable program that requires the following user input: recharge (inches/year), size of gridcell (m), land use codes for relevant time frame input as ASCII files, travel time to well input as an ASCII file, and a lookup table referencing nitrate losses from different land uses.	Program successfully created and tested against earlier spreadsheet models. For the model year 2019, spreadsheet model calculated 8.43 mg/L and the python model calculated 8.68 mg/L.

Challenges & Strategies Used to Address / Overcome:

The two primary barriers encountered during this project were a) getting a late start due to the time-lapse between the onset of the project and the acquisition of necessary computer equipment and b) identifying reliable student researchers. The first issue was noted in the mid-project review. Although most of the computers and necessary software were obtained in December 2019, that left just over half of the project period remaining. As new faculty, I sought recommendations from my colleagues for a student capable of aiding in this project. The student hired, based on those recommendations was excited about the project but in reflection, appears to have overestimated their ability to dedicate the time necessary to this project. By the time this became apparent, it was early March and COVID-19 restrictions made it difficult to identify an alternative. At that point, I decided that the best short-term course of action was to proceed on a different, but related project that could be executed in the remaining time frame by a competent programmer. I reached out to Anthony Skjellum in March 2020 and hired a student programmer based on his recommendation. The student was highly productive and able to achieve all of the desired outcomes by June 2020.

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

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

IMPACT & OUTCOMES

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

This project will have a long-term and positive impact on the career of the PI, Dr. Stephanie DeVries. Dr. DeVries is an early-career scientist and the product of this research, a program that models nitrate input to municipal water supplies as a function of land-use and groundwater flow has practical application in Wisconsin, Minnesota, Michigan, and adjacent areas where nitrate pollution is a major concern affecting the quality of water obtained from unconfined glacial aquifers. The PI anticipates at least 1 direct publication will result from this work and has already submitted abstracts to present this work at two major conferences: The Geological Society of America and the American Geophysical Union. Moreover, the program is expected to fulfill a specific need for the Wisconsin Department of Natural Resources, where it will complement an ongoing effort to develop a nitrogen management planning tool. As such, it is anticipated that the results of this project will yield additional funding opportunities to support further development of this tool. The publications, presentations, and additional funding will each have a positive impact on the PI's faculty career and potential to be awarded tenure. Moreover, these accomplishments will improve the PI's visibility in the scientific community and may create new opportunities for research collaboration.

Students Impacted

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

William (Garrett) Hooten, Computer Science ('22). Programmed a stand-alone program that calculates the concentration of a contaminant well water as a function of land use using input data from USDA CropScape and a 3D groundwater flow model. Student gained valuable experience programming a practical application and will be featured as 2nd author on resulting publications. The student is also encouraged to present his work in the 2021 Research Dialogue.

Community and Broader Impacts

The executable program developed through this project can be used by communities in Wisconsin, Minnesota, Michigan, and other regions whose municipal water supplies are derived from unconfined glacial aquifers to evaluate how changes in land use or water management influence the effective nitrate concentration in municipal water supplies. This is useful as a

forensic tool to help identify the source of high nitrates within a well capture zone but also as a planning tool to prevent or mitigate nitrate pollution in municipal wells.

Scholarly Products

Manuscripts in preparation based on the original project concept are on hold until the original work is complete.

The following technical report: DeVries, S., Bradbury, K., and Cardiff, M. “A Groundwater Flow Model for Waupaca, WI.” Wisconsin Geological Survey and Natural History Survey Technical Report was submitted for peer review on June 3, 2020. Part III of this report describes the spreadsheet-based nitrate calculator that was developed as part of the modified project goals.

A separate manuscript based on the modified project is in the early stages of preparation and is expected to be submitted to Environmental Modelling and Software (Impact Factor: 4.552) in September 2020.

Abstracts have been submitted to present this project at the Geological Society of America and American Geophysical Union Fall meetings.

An invitation to present the nitrate model to the Wisconsin Department of Natural Resources was accepted on July 1, 2020.

Inventions or Other Intellectual Property

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

Research Outreach & Collaboration

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

Bruce Rheineck, Program Manager, Drinking Water and Groundwater, Wisconsin DNR

Brian Austin, Water Supply Specialist, Drinking Water and Groundwater, Wisconsin DNR

Kenneth Bradbury, Director, Wisconsin Geologic and Natural History Survey

Paul Juckem, Hydrologist, United States Geological Survey

Michael Cardiff, Assosiate Professor, University of Wisconsin – Madison

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

EXTERNAL FUNDING

Proposal Submissions

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

Contracts/Awards Received

None to report.

Sponsored Program Capacity Building Activities

None to report

WHAT'S NEXT FOR THIS RESEARCH?

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

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

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

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

The support I received from CEACSE allowed me to set up a high-functioning workstation and remote modelling tools. Going forward, this situates me to pursue additional modelling-based research questions, including the originally proposed question of whether a Thiessen-Polygon based subsurface model is statistically comparable to more complex geologic framework models. I see continued opportunities to work with government agencies, including the

Wisconsin Department of Natural Resources and (hopefully) the Tennessee Department of Environment and Conservation to develop groundwater flow models and related resources that contribute to desired water quality and water supply outcomes.

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

N/A

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

N/A

FINANCIAL ACCOUNTING

Remaining funds include student salaries and travel. I was not able to hire students until the appropriate computer resources were purchased and some of the student salary funds went unspent as a result. Additionally, travel funds were not fully spent due to COVID-19, which led to cancellations of planned conferences in Spring 2020.

Fiscal Year 2020 Final Project Report
Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Loren Hayes, Lead PI

Other Personnel: Craig Tanis, unfunded collaborator
Project Title: Using computational approaches to enhance comparative studies of social evolution
Date Report Submitted: 1 July 2020
Award Start – End Date: August 1, 2019 – May 31, 2020
Non-Technical Summary:

Proposal aims were: (i) to streamline data collection on mammalian social organization (size, composition of social units) and mating systems (monogamy, polygamy) by developing an automated search method based on modern unstructured text extraction and machine learning techniques and (ii) produce a website where data and publications related to this research can be uploaded by the scientific community.

(i) Tanis and a student (Evan Suggs) developed an automated search platform that currently runs on a server running Ubuntu 18.04.3 LTS in the UTC SimCenter building. The backend uses Python web scraping through the packages: BeautifulSoup and Scholarly, to obtain papers from the Google Scholar database and then store their information on a local application database. This is integrated with a web application for use by researchers to mark whether the stored papers are suitable or not for a given project. This web application uses the Flask web application framework under Python 3 along with SQLalchemy for its database.

Hayes and student (Ashley Carpenter) tested this tool on several taxonomic groups for which we already had social organization data. The outcome was positive. The automated search generated the same result as the humans while saving 4 hours of effort. Carpenter, Tanis, and Hayes introduced the search tool to students in unfunded collaborator Schradin's lab (IPHC-Strasbourg, France) and Carpenter conducted literature searches using the tool for these students. Carpenter also completed a literature search on the social organization of the lagomorphs (hares, rabbits, pikas).

(ii) A group of students enrolled in CPSC 4910 (Senior Capstone Project) designed and developed a prototype outward-facing website for collecting population data relevant to this project from researchers around the globe.

The project supported the mission of the SimCenter in several ways. First, we supported student projects and an international collaboration. Hayes and Tanis recruited Dr. Jin Wang (Dept. of Mathematics) to the project and together, submitted a grant proposal to NSF. The program added a computational component to Hayes' study of mammalian social organization.

PROJECT TITLE: Using computational approaches to enhance comparative studies of social evolution

Technology Area of Interest: Health and Biological Systems

TECHNICAL APPROACH	OUTCOMES
We developed an automated search tool, permitting more efficient searches of the literature on social organization. We also developed a website template that can be used for depositing data on social organization. We also conducted searches for information on social organization and submitted a NSF IOS proposal for projects building off this funding.	(1) We determined that the automated search tool generated the same results as a human while reducing effort in the first step of data collection (searching abstract). The search tool was used to identify suitable abstracts for 657 species that had already been investigated by a human. The search required 4 hours less time than a human search. Scaled out to all mammals, this method would save approximately 30-40 hours of effort. Typically, this effort is spread over several weeks. The automated search can be run over night, reducing the number of days of effort to 1-2 days rather than several weeks. (2) We completed data collection on the social organization of lagomorphs (87 species). This information was added to Hayes and unfunded collaborator Schradin's dataset on mammalian social organization. At t he time of this report, Carpenter was running searches on other species for Schradin's students. (3) Students developed a website template that we can further develop. The website would become part of a project proposed to NSF IOS (see #4). (4) An undergrad conducted a Senior Thesis under the supervision of Dr. Craig Tanis and Dr. Joseph Dumas in late March. Section one of this thesis details

	the web application designed for use by biological research users. This section details the user interface, the database, the automated search tool, and the other technical details. Section two details experiments using machine learning and natural language processing to try and classify the papers by whether a researcher would consider them suitable or non-suitable for their purposes. The experiments ended up using document vectors in Gensim (where natural language documents are converted into a vector in a vector space) and trying to establish correlations between them using built-in models and logistic regression techniques. The final verdict was that while the document vectors were a useful data management tool, they required more substantial machine learning models to be useful as a replacement for human choice. (5) The products of this project – an automated search tool and website template – were used to bolster a grant proposal to NSF IOS (submitted in June 2020). The grant would support comparative analyses, mathematical modeling, and machine learning approaches aimed at understanding how climatic variation influences the evolution of variable social organization in mammals.
RESULTS	**OTHER INFO**
NA	*Fill in your info below.* **Budget and Schedule** * Total Budget: $17,242 Actual Used: $14,805 Balance: $2437 *spending through May 2020.

Total period of performance is 12 months.

Task 1: Months 1-6

Recruit and train students, website development, data collection.

Task 2: Months 6-12: Develop automated search tool, website development, data collection, NSF grant writing/submission.

Deliverables

- Monthly report describing numerical methods, techniques, and results that were developed or improved.

  - mid term report completed in spring 2020

- Final report detailing results, financials, and future work

  - Completed in June 2020

- Publication

  - None

- External and internal conference presentation

  Suggs, E.D. 2019. Meta-analysis in biology research literature. Association for Computing Machinery.

Organization Information

Department of Biology, Geology and Environmental Science, University of Tennessee at Chattanooga
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ACCOMPLISHMENTS & OUTCOMES

Project 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 variable social organization, despite considerable evidence that species often 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 a rate-limiting step in comparative studies because it requires manual data collection from 1000s of published papers, a process that can take researchers several months to over a year to complete. Proposal aims were: (i) to streamline data collection on mammalian social organization (size, composition of social units) and mating systems (monogamy, polygamy) by developing an automated search method based on modern unstructured text extraction and machine learning techniques and (ii) produce a website where data and publications related to this research can be uploaded by the scientific community. The PIs and two students developed and tested the effectiveness of an automated search tool that is now being used to more efficiently search for suitable abstracts on mammalian social organization. Undergraduate students taking COURSE developed a website template that with further development, could serve as a place where scientists can upload data on mammalian social organization that subsequently, can be shared broadly. A BGE undergraduate student supported by this project completed data collection on the social organization of lagomorphs (rabbits, hares, pikas) and added this information to Hayes' dataset. This student also generated suitable and unsuitable abstracts for three mammalian orders, information that was shared with the Computer Science team. A Computer Science undergraduate student conducted an Honors Thesis with Drs. Tanis and Dumas in March 2020. The thesis focused on web application design and experiments using machine learning and natural learning processing to classify papers as suitable or unsuitable. PI Hayes met with NSF program officers to discuss a proposal related this project. Hayes and Tanis and new collaborator Wang (Mathematics) submitted a proposal to NSF IOS.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Develop automated search tool	A search program was developed and tested; modifications are being made
Website development	Template developed
NSF grant proposal development	Proposal submitted to NSF IOS

New collaborator	Jin Wang joined the collaboration and will lead a mathematical modeling project pending NSF funding
Student training	The PIs trained 1 BGE undergrad and 4 Eng/CS undergrads

Challenges & Strategies Used to Address / Overcome:

The website development project, while beneficial to students, did not progress as far as we had hoped. Future work will need to focus on a user-friendly spreadsheet similar to a Google Docs or online Excel document format.

The coronavirus pandemic impacted our schedules and ability to work cohesively. Despite this, we held regular meetings in spring 2020 and shifted some priorities in budget spending e.g., purchasing books that we will need going forward rather than publication costs.

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

The initial implementation of our abstract screening web application only works with Google Scholar through an unofficial Python package called Scholarly. The nature of this Google Scholar data and the dependency on web formatting choices made by Google makes this particular implementation somewhat limited and fragile. A longer term goal is to integrate the web application with the Web of Science database, and indeed the application is designed to have modular support for arbitrary backend data providers, but access to the full Web of Science API is cost-prohibitive at this point.

IMPACT & OUTCOMES

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

Loren Hayes: This project was critical to the development of Hayes' and unfunded collaborator Schradin's collaborative study on mammalian social organization. The automated search tool has already been used for searches on some taxonomic groups. The machine leraning framework developed by Tanis is part of a continuation study of how rainfall impacts the evolution of variable social organization – funded by CEACSE. The framework and tools that Hayes and Tanis developed bolstered a NSF grant proposal submitted in June 2020. If funded, we will be able to hire the personnel necessary to complete long-term project goals.

Craig Tanis: This work offers Dr. Tanis the opportunity to leverage his system design and internet application expertise, and to further develop local expertise in Machine Learning and Biology research, potentially benefiting other SimCenter thrust areas.

Students Impacted

Evan Suggs (Engineering and Computer Science, graduated May 2020): Evan worked as an hourly researcher on the project. He developed an automated search tool and worked on a senior thesis project on machine learning. His graduate work will be supported by Hayes and Tanis' full CEACSE award.

Ashley Carpenter (BGE, graduated May 2020): Ashley worked as an hourly researcher on the project. She conducted a validation study of the automated search tool for three taxonomic groups, showing that the method was effective at reducing effort. She also collected social organization data on the lagomorphs (rabbits, hares, pikas) and helped train French students using the search tool.

Harold Hansen, Carter Hill, Parshwa Patel & Bowen Wexler (Engineering and Computer Science, graduated in 2020): These students developed a website template for our project to partially fulfill the requirements for CPSC 4910.

Community and Broader Impacts

The mini-CEACSE funding allowed the PIs to develop a strong collaboration and build a foundation for future study. The research conducted with the support of CEACSE is intimately linked to Hayes' research on social mammals and a NSF IOS proposal submitted by Hayes and Tanis in June 2020. That proposal outlines several important goals made possible by the initial CEACSE funding:

- **This will be the first comparative study to determine how environmental quality at the population level shapes social evolution within populations. This information is critical to predicting species resilience to environmental change.** Changes in social organization due to environmental disruption and/or demographic events could negatively impact the stability of social interactions and reproductive success of some group members. Alternatively, flexible social strategies may permit some species to acclimate to a changing climate. Non-reversible mechanisms leading to VSO can lead to speciation. Thus, predictions on environmental conditions favoring different factors leading to VSO (Obj. 3) will improve understanding of population processes enhancing biodiversity and inform wildlife management and conservation strategies.

- **Our dataset will be high quality, expandable, and accessible.** We will produce publications comparing reported social organizations and life history traits in our dataset vs. other datasets, to demonstrate the benefits of taking a methodical approach to building a dataset. Other social and life history data can be added in the future, allowing for additional hypothesis testing beyond the scope of this study. Making the dataset accessible online, and expandable, will promote its widespread use.

Mini-CEACSE funding also permitted the development of new Broader Impacts activities described in our NSF IOS proposal, including:

***Working group*:** Effective conservation strategies require input from a diversity of partners, including behavioral ecologists. Effective species management strategies need to account for the possibility that species with VSO may be better "equipped" to respond to environmental perturbations. Thus, we will culminate the project with a 3-day working group at the UTC SimCenter. The aim of the working group will be to inform wildlife managers (local and Tennessee state wildlife managers will be invited) about the results of the proposed study. Discussion will focus on how the data can inform effective wildlife conservation and management strategies that account for intraspecific variation and to learn what kinds of additional data wildlife managers need in the future. *Follow-up*: We anticipate that participants will (i) collaborate on a paper and/or conference symposium on intraspecific variation and conservation and (ii) develop guidelines for conservation and management practices for state and federal wildlife agencies.

Scholarly Products

Publications:

1. None, yet.

External Conferences:

1. Suggs, E. 2019. Meta-analysis in biology research literature. Association for Computing Machinery.

Presentations at UTC:

1. Carpenter, Hayes and Tanis presented (via Zoom) the automated search tool to unfunded collaborator Schradin's lab group at IPHC-Strasbourg, France. The presentation was informal and aimed to teach the researchers how to use the tool to search the literature for suitable abstracts.

Inventions or Other Intellectual Property
None

Research Outreach & Collaboration

Hayes and Tanis recruited Dr. Jin Wang (Mathematics) to the collaboration. Together, they submitted a grant proposal to NSF Integrative Organismal Systems (IOS). The proposal aims are to (i) extend the dataset developed in part during this study, (ii) use comparative and machine learning approaches to estimate how climatic variation influences the evolution of social organization, and (iii) use mathematical modeling to predict how climatic variation influences factors leading to variable social organization.

EXTERNAL FUNDING

Proposal Submissions

1. **FY2020-2021 Center of Excellence in Applied Computational Science & Engineering (CEACSE)**: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models (co-PI, Dr. Craig Tanis, UTC College of Engineering). Funding: $98,662.
2. **National Science Foundation:** Comparative and computational analyses of climatic and life history drivers of variable social organization in mammals. (PI: Loren Hayes, co-PIs Craig Tanis & Jin Wang, $610,809). Proposal no. 2037549, submitted in June 2020.

Contracts/Awards Received

1. **FY2020-2021 Center of Excellence in Applied Computational Science & Engineering (CEACSE)**: Climate and social evolution: Using machine learning to improve dataset quality and to develop predictive models (co-PI, Dr. Craig Tanis, UTC College of Engineering). Funding: $98,662.
2. **National Science Foundation** (#1854177): Collaborative Research: IRES Track I: Stronger together: Exploring how communal care reduces individual costs during challenging years (2019-2022; **PI: Loren Hayes**; co-PIs, Shewanee Howard-Baptiste, & Jennifer Ellis). Funding: $263,356 (In collaboration with Dr. Carolyn Bauer, total award = $399,968). Note: This award was made in August 2019. Although not directly related to the project, it is possible that I could use this funding to support computational work with collaborators in Chile.

Sponsored Program Capacity Building Activities

1. Hayes met with NSF IOS and OISE program officers at NSF offices (Virginia) in February 2020.

WHAT'S NEXT FOR THIS RESEARCH?

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

Over the next 3-5 years, Hayes and unfunded collaborator Schradin's research groups will use the tools developed by this grant to extend a dataset on mammalian social organization. In Fall 2020, two graduate students (1 CS, 1 BGE, supported by a full CEACSE grant to Hayes and Tanis) and a BGE undergraduate student will (i) collect data on rainfall and life history factors that could influence the evolution of social organization and (ii) use machine learning to model the effects of variable rainfall on the evolution of variable social organization. The automated search tool will be used by French students to search the literature for suitable abstracts on social organization. Pending NSF funding, the project could extend to 5-6 years, permitting the publication of papers on social organization, the use of computational tools to inform behavioral ecology studies, and an analysis of how climate influences social evolution.

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

CEACSE funding gave Hayes the tools and flexibility to develop a computational study of mammalian social organization. The full CEACSE grant to Hayes and Tanis will support the development of machine learning tools to model the effects of rainfall on the evolution of social organization. In this way, the CEACSE funding has broadened the ways that Hayes can understand how the climate influences social organization in mammals. Pending NSF funding, Hayes, Tanis, and Wang will extend a dataset on terrestrial mammal social organization that includes information on (i) variation in social organization (VSO) within populations, (ii) reversible (social flexibility, developmental plasticity) and non-reversible (environmental disruption, genetic differentiation) factors leading to VSO, and (iii) climatic and life history (lifespan, breeding attempts) data. The PIs will build machine learning models to predict the presence of VSO in representative taxonomic groups based on predictability of rainfall and temperature, providing a framework for comparative analyses and mathematical modeling. Using Bayesian mixed-effects phylogenetic models, the PIs will estimate the ancestral social state and test hypotheses for how rainfall, temperature, and life history affected transitions to other social organizations, including VSO. Mathematical modeling will be used to predict the influence of these climatic conditions on reversible and non-reversible factors leading to VSO.

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

The computational elements of this study will broaden an already successful project on mammalian social organization. In Spring 2020, a related paper on Artiodactyla social organization was published in a high impact journal, indicating the potential for future high-profile publications.

Jaeggi, A., Miles, M.*, Festa-Bianchet, M., Schradin, C., & **Hayes, L.D.** Variable social organisation is ubiquitous in Artiodactyla and readily evolved from pair-living ancestors. *Proceeding of the Royal Society B*. https://doi.org/10.1098/rspb.2020.0035. Impact factor: 4.304

What barriers (if any) do you face to reach these next goals?
The main barrier to future success is funding. We need funding to support Masters projects, a postdoc, and the PIs own efforts. The full CEACSE grant that Hayes and Tanis hold will allow for some progress. However, NSF IOS funding is highly competitive. That said, the PIs will have support through CEACSE to develop another proposal should their current submission not be funded.

FINANCIAL ACCOUNTING

We did not publish a paper, yet. Thus, we reallocated some funds from publication costs to supplies. We purchased two textbooks on machine learning/statistics and a comprehensive book on cetaceans. The former will be used by a graduate student to develop a framework for machine learning studies. The latter will be used by BGE/ESC students to inform a paper on cetacean social organization.

Fiscal Year 2020 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Ashley Manning-Berg, Lead PI

Other Personnel: N/A

Project Title: Modeling of microbial mat decay and implications for the early Earth fossil record

Date Report Submitted: July 1, 2020

Award Start – End Date: August 1, 2019 – May 31, 2020

Non-Technical Summary:

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

The project is still on-going and has been extended into the 2020-2021 fiscal year. During the 2019-2020 year, I have compiled code that was used in previous publications and began to work with Drs. Skjellum and Arabshahi in the SIMcenter to recreate the code that is currently in multiple coding languages. I have also reached out to other potential collaborators on campus and inquired about getting a student involved in the project to help move the coding forward. I have also been researching possible decay pathways that organisms may take as they undergo decomposition and will work with the SIMcenter and students to model decomposition when the mat model has been built.

PROJECT TITLE: Modeling of microbial mat decay and implications for the early Earth fossil record

Technology Area of Interest: Health & Biological Systems

PROPOSED TECHNICAL APPROACH	OUTCOMES
• Reconstruct the microbial mat model that has been used in previous publications. • Incorporate decomposition into the model	• Will result in a code published on GitHub • Decomposition model will either lead to publication or serve as the basis for an external grant proposal.
RESULTS	**OTHER INFO**
	Budget and Schedule Total Budget: $15,000 Actual Used: $2,300.09 Balance: $12,699.91 Total period of performance is 12 months. Task 1: Months 1-6 – get model up and runing Task 2: Months 3-6 - figure out how to incorporate decomposition into the model Task 3: Months 6-12 - analyze the model Task 3: Months 8-12 – write a paper **Deliverables** • Mid-term report

ACCOMPLISHMENTS & OUTCOMES

Project Overview

Microbial mats are organic structures that represent Earth's earliest ecosystems. Evidence for ancient microbial life can be found in 3.5 billion-year-old rocks, and in most cases, evidence is based solely on the morphology of the fossil. Many of the best fossils are preserved in rocks that would require rapid mineral precipitation early in the rock forming process before the microorganisms were significantly altered by decomposition. Taphonomic laboratory studies grow monocultures of cyanobacteria that are analogous to the cyanobacteria found in the fossil record and monitor changes to the morphologies of the organisms as they decompose. However, the effects of decomposition on microbial mat preservation are unknown because growing microbial mats in a lab is difficult and time consuming.

Previous microbial mat models that incorporate chemical gradients and the interaction between the various microbial communities found in mats will be used to "grow" biomass in each microbial community. The first step of this modeling study will be to solve the model to obtain a biomass value. That biomass value will be used to model decomposition using the differential equations that describe constant decay, time-wise decay, and predator-prey relationships, and provide insight to how biomass will change over time in these scenarios. Once the relationship between biomass and time is established, the biomass values will be compared to models based on laboratory experiments to predict the percentage of the biomass that would be well-preserved versus poorly-preserved, ultimately predicting what the fossil assemblage would look like given a specified time that the organisms were exposed to decomposition prior to fossilization.

This research will model microbial mat decay over time and use that model to predict the range of microfossil morphologies that would be observed in the rock record. Biomass accumulation within a mat will be calculated using a previously developed model and used in decomposition models to establish a relationship between biomass and time. The quality of microbial preservation can then be predicted based on the amount of time the mat was exposed to decomposition.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Reconstruct the microbial mat model	Working on getting a student to help with this.
Identify decomposition pathways	Writing a paper with another collaborator to do this (Excel based, simple math model)
Incorporate decomposition models into the mat model	Ideally, this will provide a sense of timing for preserving a microbial mat that we can determine based on the taphonomy preserved
Write a paper	
Use this to apply for funding using a real mat	

Challenges & Strategies Used to Address / Overcome:

I was challenged by my higher course load, with 3 and 2 new preps during my first year of teaching. The transition to online instruction was also a challenge. While I will have the same course load in my second year of teaching, I am hopeful that I will be able to overcome the challenge.

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

This was a tough year to get this work accomplished. With my teaching load and the effects of COVID-19 on the university, I struggled to get the work accomplished. I am also unfamiliar with modeling languages and the modeling techniques used to create the original mat model and therefore am reliant on the help from the SIMcenter. I am hoping to find some modeling classes to take over July so that I can be better prepared and able to understand the model better.

IMPACT & OUTCOMES

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

When complete, this project will help me to have collaborators across the UTC campus, and will be presented at conferences in my discipline. It has also helped me establish a relationship with the SIMcenter.

Students Impacted

I am still working to find a student to help with the modeling.

Community and Broader Impacts

This research will help the geobiology community to interpret taphonomic changes to microorganisms when they are behaving in a consortium, which is what we expect to happen in a natural system.

Scholarly Products

Publications:

1. N/A at this time.

External Conferences:

1. N/A at this time.

Presentations at UTC:

1. N/A at this time.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

I am hoping to collaborate with the mathematics department at UTC to help with the modeling. I will build on my current collaboration with a colleague at Gustavus Adolphus College in St. Peter, MN, who has been working with me to develop the decomposition pathways models for individual species.

EXTERNAL FUNDING

Proposal Submissions

1. N/A at this time

Contracts/Awards Received

1. N/A

Sponsored Program Capacity Building Activities

1. N/A

WHAT'S NEXT FOR THIS RESEARCH?

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

Over the next year, I will finish the work that I have outlined in my proposal. Once the model is made, I would like to start a laboratory-based actualistic experiment observing changes to a microbial mat to see if the model is correct. It takes several years to grow and monitor a microbial mat so this will be a project that will run in the background of my lab for several (~5 to 7 years). I will also compare the model to several well-preserved examples in the rock record to see if the model is able to provide any information regarding the timing of decomposition prior to the lithification of the rock.

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

I will work with each of the collaborators in the future. I'd like to start working on a image analysis project tat uses a high-resolution image as a map for geochemical analyses and will need support from the SIMcenter to do that work.

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

N/A

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

My biggest barriers right now, are my personal knowledge of how to use or create a model; however, I am collaborating with people who do understand the modeling aspect. The other concern I have is my course load for the upcoming year, especially with the transition to online learning again. I'm hopeful that I will be able to move the project forward despite the challenge.

FINANCIAL ACCOUNTING

The funding that remains is being carried over to the 2020-2021 fiscal year. Much of the help that I have received from the SIMcenter has been free and I am working to find a student to start working on the project, which will spend the money budgeted. I have already purchased a laptop; however, will have to return it because the hardware was faulty when it arrived. I will purchase another one. Some of the money has been spent toward my summer salary while I have been researching decomposition pathways.

Fiscal Year 2020 Final Project Report

Tennessee Higher Education Commission: Center of Excellence in Computational Science and Engineering Grant Competition (Faculty Initiation and Career Opportunity Award)

Dr. Reetesh Ranjan, Lead PI

Other Personnel: N/A

Project Title: A multi-fidelity computational modeling strategy for large-eddy simulation of turbulent combustion

Date Report Submitted: 6/29/2020

Award Start – End Date: September 1, 2019 – May 31, 2020

Non-Technical Summary:

The research project focused on the development and demonstration of a multi-fidelity computational modeling framework for the study of chemically reacting turbulent flows. Such flows also referred to as turbulent combustion, are observed in energy conversion and rocket propulsion devices. The multi-fidelity approach comprises of three strategies, namely, a high-fidelity direct numerical simulation (DNS) technique for fundamental investigation of flame-turbulence interactions, a large-eddy simulation (LES) based modeling approach for efficient investigation of practical applications, and a nonlinear reduced-order modeling (ROM) strategy for simulation-based design evaluations. The key objectives of the project include establishing the nonlinear ROM for LES of turbulent flows, development, and assessment of a modular and efficient multi-scale subgrid models for turbulent combustion, and evaluation of the opensource software OpenFOAM for high-fidelity numerical investigation of turbulent flows. All these objectives have been addressed under this project, which has led to the development of an in-house parallel fully compressible reacting flow solver with advanced subgrid models and ROM capabilities.

The research work under this project has resulted in a verified and validated computational modeling framework with predictive capabilities that can be used for high-fidelity investigation of chemically reacting turbulent flows through LES and nonlinear ROM. It has trained students in the use of high-performance computing resources at SimCenter for the study of chemically reacting turbulent flows. It has further helped the PI to maintain active collaboration with the Georgia Institute of Technology and established newer internal and external research collaborations. The work under this project expands the current research capabilities of SimCenter in the area of combustion, reduced-order modeling, data-driven modeling, and multi-scale modeling. The outcomes of the research are published in the form of conference articles and presented at internal and external conferences. Finally, several white papers and proposals leveraging the result from this work have been developed for seeking external funding to further extend the work.

PROJECT TITLE: A multi-fidelity computational modeling strategy for large-eddy simulation of turbulent combustion

Technology Area of Interest: Turbulent Combustion

TECHNICAL APPROACH

Development and assessment of multi-fidelity approach for turbulent combustion

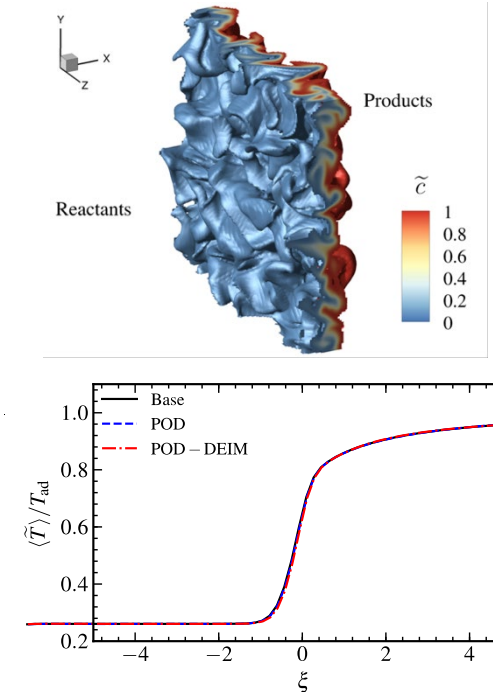
- High-fidelity and nonlinear reduced-order modeling (ROM) computational tools
- Implementation and assessment of ROM tools in a multiphysics flow solver
- Improvement of multi-scale subgrid-scale (SGS) models
- Verification and validation studies
- Evaluation of OpenFOAM for non-reacting and reacting flows

OUTCOMES

A validated multi-fidelity computational framework for study of turbulent combustion

- Results presented at AIAA SciTech and Research Dialogues at UTC.
- Published a conference paper, another conference paper is in review and a journal paper is being written up.
- Trained UG students for usage of SimCenter resources.
- Setup of a new computing server and
- Established an agreement with Georgia Tech to use their combustion code.

RESULTS



Flame brush of a turbulent premixed flame within the thin reaction zone regime (a) and normalized temperature profile comparing results from ROM approaches with reference solution (b).

OTHER INFO

Budget and Schedule

Total Budget:	$25,000
Actual Used:	$21,027.44
Balance:	$3,172.56

Total period of performance is 10 months.

Task 1 (Months 1-3): Development of nonlinear ROM tools and SGS models

Task 2 (Months 4-7): Verification and validation studies and OpenFOAM evaluation

Task 3 (Months 8-10): Verification of OpenFOAM and assessment of SGS models

Deliverables

- Established multi-fidelity computational framework for turbulent combustion
- Assessment of OpenFOAM for investigation of turbulent flows
- Publications and conference presentations
- Mid-term and final reports

Organization Information

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ACCOMPLISHMENTS & OUTCOMES

Project Overview

Background: Chemically reacting flows observed in energy conversion and propulsion devices are turbulent, multi-physics, and multi-phase in nature. The added complexity of chemical reactions to turbulence makes a computational investigation of such flows extremely challenging. While direct numerical simulation (DNS) helps to gain a fundamental understanding of turbulence-chemistry interactions, it becomes computationally prohibitive for practical applications. To this end, large-eddy simulation (LES) is a promising approach, where the large-scales of motion are explicitly resolved, and the effects of the unresolved small-scales of motion are modeled by using subgrid-scale (SGS) closures. Although LES coupled with the use of high-performance computing (HPC) provides efficient means for studying practical systems, the SGS modeling still has several limitations. Additionally, LES still tends to be computationally expensive for simulation-based design, thus requiring the use of high-fidelity reduced-order modeling (ROM) approaches. This research effort focused on establishing a multi-fidelity computational framework for the investigation of turbulent combustion. The multi-fidelity strategy comprises of three techniques, namely, a high-fidelity DNS approach, a physics-based multi-scale subgrid modeling approach, and a nonlinear ROM approach. The multi-scale subgrid model for LES of turbulent combustion also referred to as RRLES, provides the filtered reaction-rate (a key quantity for modeling of turbulent combustion) by using the linear eddy mixing (LEM) model at the subgrid level in conjunction with an adaptive mesh refinement (AMR) technique. The nonlinear ROM utilized proper orthogonal decomposition (POD) modes as basis functions for a Galerkin projection, and the discrete empirical interpolation method (DEIM) was used for efficient computation of the nonlinear terms. The work conducted under this research effort addressed the challenges associated with both these approaches.

Scientific Aims: The key objectives of the research work include: (a) Improvements to physics-based modeling capabilities of RRLES, (b) establishing the nonlinear ROM approach for reacting flows, (c) Establishing a modular approach for SGS closure of turbulent combustion, and (d) evaluation of capabilities of the OpenFOAM software framework.

Methodologies/Activities: The objectives of the research were accomplished through several activities. The capabilities of the multi-scale subgrid model for turbulent combustion was improved by employing a locally patch-based dual-grid approach to emulate the multi-level AMR framework. The accuracy, stability, and computational efficiency aspects of the nonlinear ROM strategy was examined through a canonical turbulent premixed flame configuration. The implementation was improved further to reduce the computational memory footprint. Finally, the capabilities of OpenFOAM for simulation of a wide range of turbulent flows were comprehensively assessed through several canonical and complex test cases.

Outcomes: The research work has resulted in a verified and validated computational modeling framework with predictive capabilities that can be used for high-fidelity investigation of chemically reacting turbulent flows through LES and nonlinear ROM. It has trained students in the use of HPC resources for simulation of chemically reacting turbulent flows. Furthermore, the outcomes of the research activities are published in the form of conference articles and presented at internal and external conferences. Finally, several white papers and proposals leveraging the result from this work have been developed for seeking external funding to further extend the work.

List of Objectives / Aims / Major Milestones Proposed	Cumulative Outcomes / Accomplishments
Development and assessment of nonlinear ROM tools for turbulent combustion	Established the nonlinear ROM and performed comprehensive verification study by considering turbulent premixed flames
Multi-scale modeling of turbulent combustion	The physics-based modeling capability has been enhanced further
Establish a modular approach and evaluate acceleration technique	Implemented approaches for modularity and portability of algorithms to hybrid computing architectures
Evaluate capabilities of OpenFOAM	Comprehensive assessment of OpenFOAM was performed through a series of test cases

Challenges & Strategies Used to Address / Overcome:

A major challenge faced by the PI was related to student engagement. As a new faculty member, it was difficult to find students. Furthermore, the research topic was highly specialized. Therefore, it required a substantial amount of training, particularly for undergraduate (UG) students. Since there were only UG students involved in this project, the progress on the publication front was slower than anticipated.

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

While the baseline nonlinear ROM strategy worked on fundamental problems, under certain operating conditions and for complex geometries, numerical instabilities were observed. Some of the other recent studies have observed similar issues with nonlinear ROM of different class of problems. Therefore, further work is needed to examine the issues so that robustness of the method can be improved further.

IMPACT & OUTCOMES

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

This initiation project has impacted the career of the PI on many levels. Firstly, it has helped in setting up of the Fluids and Combustion Modeling (FCM) research group at the University of Tennessee at Chattanooga (UTC) by providing support for high-performance computing resources, establishing advanced computational tools, travel to conferences of international repute, and engaging UG students in state-of-the-art research. All these activities have assisted the PI in showcasing the novel computational modeling capabilities developed within the FCM research group, where the focus is on the development of multi-fidelity methods and physics-based models for numerical investigation of multi-physics turbulent flows. It has also led to the strengthening of the ongoing research collaboration of the PI with the researchers from the Georgia Institute of Technology (GT) and established newer collaborations. Furthermore, the project outcomes have allowed the PI to develop multiple white papers and proposals seeking extramural funding. The project has also helped the PI in enhancing project management and mentorship skills.

Students Impacted

Under this project, two UG students were trained who contributed to the research activities. The specific details are given below:

1. **Ashwyn Sam:** He was first trained to use visualization software tools such as Paraview and Tecplot and Python for data analysis. Afterward, he learned to initialize isotropic turbulence using an in-house software referred to as TurbInit. Afterward, he was trained to solve laminar premixed flame configuration using Cantera. He set up and analyzed the turbulent premixed flame problem in physical and spectral space using Python-based tools. Also, he learned to conduct high-fidelity fundamental turbulent combustion simulations using high-performance computing (HPC) resources at SimCenter and assessed the performance of OpenFOAM software for simulation of reacting and non-reacting flows. Finally, he was mentored on the essence of collaborative research and technical presentation and reporting skills.
2. **Brennan Troxel:** He was also initially trained for different software and computational tools such as Paraview, Pointwise, Python, etc. Afterward, he focused on the generation of computational mesh for LES of the established VOLVO combustor. In parallel, he learned the OpenFOAM software. After going through several tutorials, he set up the VOLVO case from scratch by following a published research article. He also got trained on the use of HPC resources at SimCenter and to perform scaling analysis for parallel computing. He ran the no-reacting flow within the VOLVO rig and documented all his findings in the form of weekly research presentations and mid-year and final reports.

Community and Broader Impacts

The activities conducted under the projects have broader impacts at various levels. The demonstration of the computational tools has established the predictive capabilities for investigation of practically relevant turbulent combustion so that such a framework can be used by a community of researchers focused on the development and application of data-driven modeling. The PI has worked closely with UG students at UTC, which has prepared them for solving challenging problems associated with the design and evaluation of combustion devices by using novel and advanced computational tools. The research work has also featured the use of HPC resources facilitated by the SimCenter at UTC to conduct high-fidelity investigations of reacting turbulent flows. Finally, the outcomes of the research activities have been presented at the AIAA SciTech Forum and Exposition 2020, which has showcased the computational research capabilities of UTC.

Scholarly Products

Software:

1. **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. Under an agreement between the PI and Prof. Menon, the code can be used by the members of the research group directed by the PI at UTC to conduct independent research activities. The newer capabilities developed at UTC will be shared with CCL at GT for collaborative research.

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

Publications:

1. R. Ranjan, and S. Menon, “Application of Nonlinear Reduced Order Modeling Strategy for Large Eddy Simulation of Chemically Reacting Turbulent Flows”, AIAA-2020-2140, AIAA SciTech Forum and Exposition, 2020. (DOI: https://doi.org/10.2514/6.2020-2140)
2. Assessment of Two Level Simulation Model for Compressible Turbulent Mixing Layer, Accepted**,** 17th International Workshop on the Physics of Compressible Turbulent Mixing, Atlanta, USA, July 13-17, 2020.
3. Application of Hybrid Transported-Tabulated Chemistry for Efficient Large-Eddy Simulation of Turbulent Premixed Combustion, Under Review, AIAA SciTech Forum and Exposition, 2021.

External Conferences:

1. AIAA SciTech Forum and Exposition, 2020, Orlando, FL, USA.

Presentations at UTC:

1. R. Ranjan, “Application of reduced order modeling for simulation of turbulent combustion”, Research Dialogues, 2020.

Inventions or Other Intellectual Property

N/A

Research Outreach & Collaboration

The research work conducted under this project has led to both internal and external collaborations. Such collaborations have led to the development of internal and external proposals and white papers. The list of collaborators is as follows:

1. Dr. A. Arabshahi, SimCenter, UTC.
2. Dr. K. Sreeenivas, Mechanical Engineering, UTC.
3. Dr. O. A. Osman, Civil Engineering, UTC.
4. Dr. E. Kaplanoglu, Engineering Management & Technology, UTC.
5. Dr. J. Sethi, UT College of Medicine.
6. Dr. S. Menon, GT.
7. Dr. V. R. Hasti, Prudue University.

EXTERNAL FUNDING

Proposal Submissions

Following white papers and proposals have been submitted related to this award

1. A Data-Driven Multi-Parameter Reduced Order Modeling Framework for Investigation of Hypersonic Systems (**White Paper**, AFOSR # FOA-AFRL-AFOSR-2020-0002, Topic #26)
2. An Integrated Approach for Characterization and Predictive Modeling of Non-Equilibrium High Speed Turbulent Reacting Flows (**White Paper**, ONR Announcement # N00014-20-S-F003, Topic #9)

3. Low Emission combustor system for high overall pressure ratio compact core engines (**Stage A Proposal**, NASA ULI, Ultra-Efficient Subsonic Transports, Strategic Thrust 3)
4. Modeling Impact of Wind Turbulence on Autonomous Vehicles (**Proposal**, One UT Collaboration & Innovation Grant)
5. COVID-19-Relevant Computational Modeling of Human Respiratory Airways (**Proposal**, DOD IIRA W81XWH-20-PRMRP-IIRA-COV)

Contracts/Awards Received

None

Sponsored Program Capacity Building Activities

1. Attended the NSF CAREER proposal webinar.

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 has been leveraging the outcomes of this project work to seek extramural funding in the areas of turbulent combustion, data-driven modeling, reduce order modeling, and turbulence modeling, and will continue doing so in the future. In addition, further developments and improvements to the established approach will be performed in the future. The technical capabilities developed under this effort complement the existing capabilities of researchers at SimCenter, which will allow the PI to seek collaborative external research funding. The tools developed under this project have been documented and archived so that the new generation of students can be easily trained. Finally, the ongoing collaboration with Georgia Tech enables further research opportunities and can potentially be used for engaging exchange students.

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

The support received from the CEACSE although focused on computational modeling of turbulent combustion, it has established different tools such as chemistry modeling using Cantera, evaluation of OpenFOAM for simulation of non-reacting and reacting flows, and particle-laden turbulent flows. The project has already helped in pursuing an investigation of biomedical flows using OpenFOAM and advanced subgrid models for turbulent flows. The support has allowed the PI to develop both internal and external research proposals and will enable such activities in the future.

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

None

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

None

FINANCIAL ACCOUNTING

Currently, the project has $3,172.56 of remaining funds, which is related to the staff benefits. Based on the approval from SimCenter, these funds will be used to support an UG student during the summer to further extend the current research.