

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 2015-2016**

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EXECUTIVE SUMMARY

UTC's Center of Excellence in Applied Computational Science and Engineering (CEACSE) is embarking on a new 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 FY2015, CEACSE marked its first decade of existence, 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 FY2016 documents focused priority areas, a visionary leadership team, and greater impacts across a range of stakeholder groups.

CEACSE activities enhance education at all academic levels including through the Ph.D. program in Computational Science. Graduate and undergraduate students have participated in various research activities undertaken as a result of CEACSE funding. Because of those research activities, area companies continue to have interest in the educational programs impacted by CEACSE initiatives. In the current year the College of Engineering and Computer Science (CECS) and the SimCenter will broaden efforts to partner with companies in the Chattanooga region and beyond. Because of increasing capabilities in high-performance computing and the growing importance of modeling, simulation, and advanced computing in research and education, the efforts of our researchers will continue to serve as research anchors attracting students from across the nation and internationally.

CECS and the SIM Center continue to foster a 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 their educational and other academic milestones of performance, and we are providing increased support through the Office of Research and Sponsored Programs, through focus on opportunities that can lead to larger funding awards, and through development of strategic partnerships.

The following is the Annual Report for Fiscal Year 2016 of CEACSE activities and efforts. On behalf of the University of Tennessee at Chattanooga, the College of Engineering and Computer Science, the SIM Center, and the Center's community partners, we express our appreciation to THEC for critically important support of the CEACSE.

INTRODUCTION

The value proposition for cross-disciplinary research, education, and training in the rapidly advancing field of Computational Science and Engineering¹ (CSE) has grown stronger since the start of CEACSE in 2005. Today, modeling, simulation and high-performance computing 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 to:

- Expand CSE capabilities at UTC;
- Support start-up 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.

Fiscal year 2016 has been a year of transition for CEACSE. After several retirements and resignations of staff in the SimCenter, the appointment of new leadership has revitalized the environment for CEACSE at UTC. Dr. Reinhold Mann was appointed as the Interim Director for the SimCenter; Dr. Joanne Romagni was appointed as the new Vice Chancellor for Research and Dean of the Graduate School; and Dr. Daniel Pack was appointed as Dean for the College of Engineering and Computer Science. This new leadership team has articulated a vision and developed a strategic plan for the SimCenter that includes broad engagement of cross-disciplinary faculty. Additionally, a search for a new SimCenter Director and Chair of Excellence in CSE is underway at the time of submission of this report. This position will direct the CEACSE program and report, via the Vice Chancellor for Research, to the UTC Chancellor as laid out in the original CEACSE proposal.

The FY2016 portfolio of CEACSE projects accomplished a number of foundational advancements in solving complex systems of partial differential equations (PDE) in space and time, and also expanded CSE capabilities in important new application areas such as modeling and simulation of acoustic metamaterials and energy efficiency in turbo-machinery.

Much effort in FY2016 was focused on developing a path forward for modernizing the high-performance computing infrastructure at UTC that serves the CSE research and graduate training efforts. As a result, UTC will make an investment in FY2017 to modernize the current HPC cluster, and continue to work the collaborative relationships with the Leadership Computing Facility (LCF) at the Oak Ridge National Laboratory (ORNL), and with the UT/ORNL Joint Institute of Computational Sciences (JICS).

¹ “Future Directions in CSE Education and Research,” report from workshop sponsored by SIAM and the European Exascale Software Initiative (EESI-2), held August 4-6, 2014; Breckenridge, CO – Draft, dated March 11, 2015 available at <http://www.eu-maths-in.eu/download/General-International-Studies-Prospective/2015-CSE-report-draft.pdf>.

CEACSE 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. Figure 1 (below) illustrates the central role CEACSE plays in capability and program development potentially affecting all Colleges at UTC. These strategies intersect with problems of global, national and regional importance in five primary focus areas:

- Aerospace and Defense
- Energy & Environment
- Health & Biological Systems
- Manufacturing
- Urban Science and Technology

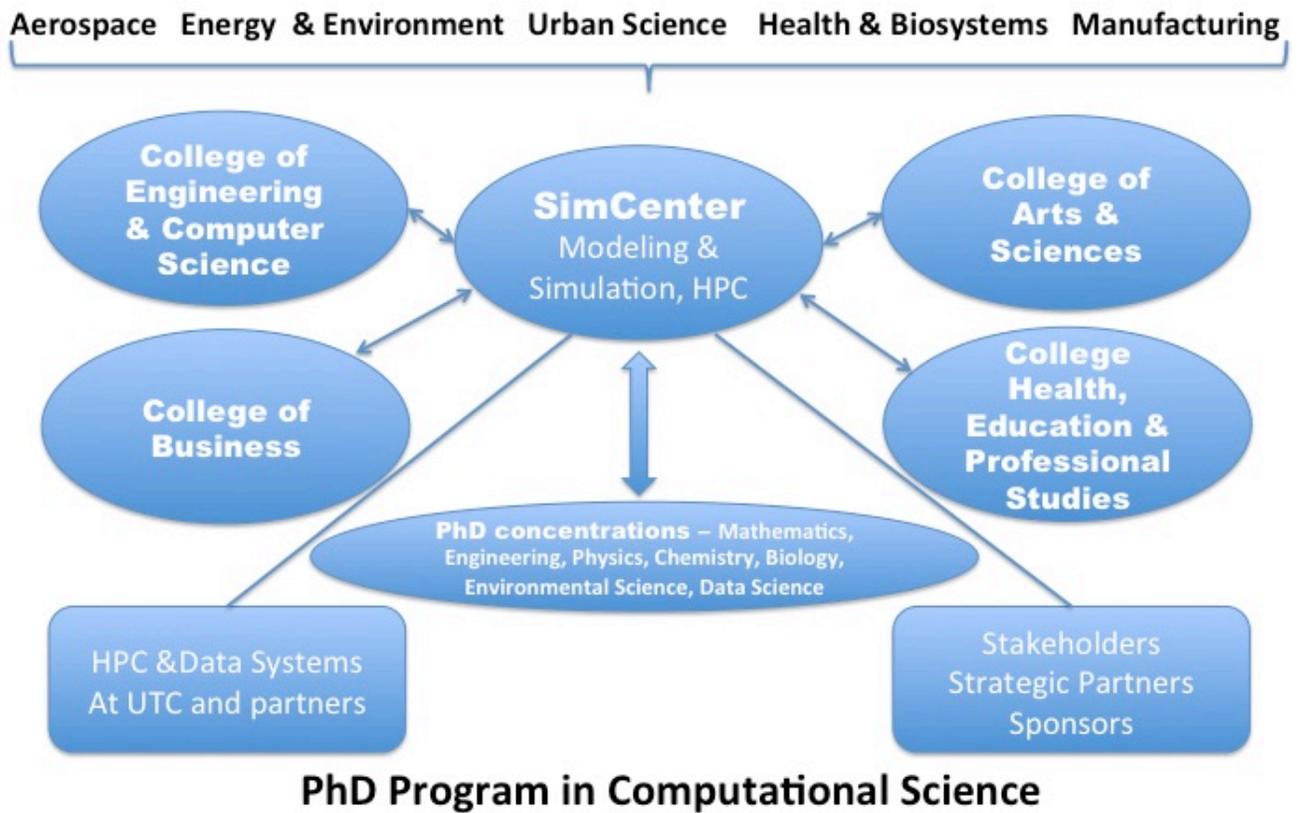
These application focus areas were selected based on three important criteria:

- The presence of significant scientific and technical challenges for which there was interest and expertise at UTC;
- Clear alignment with educational and workforce development missions of UTC;
- 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 one of these five focus areas are reviewed for technical merit by a panel of outside experts, then undergo a review for strategic alignment which includes scrutiny of a specific plan to develop extramural funding. While these five focus areas span a wide area of science & technology, all excellent ideas that appear outside of these areas are considered, as long as they have substantial CSE content.

Figure 1: SimCenter serves as a hub in modeling, simulation and HPC in collaboration with departments across UTC. Drivers for the activities include the five focus areas described in this plan. In addition to Computer science and Engineering, the PhD program will feature concentrations in Mathematics and other Sciences. The THEC Center of Excellence supports cross-disciplinary innovative efforts that are critically important to continued program development.

Center of Excellence in Applied Computational Science and Engineering at UTC



2016 PROJECTS AND FUNDING

In FY16, CEACSE awarded new seed funding to support the research activities of twelve faculty members for seventeen new projects from various disciplines, including computational engineering, computer science, engineering, business, and mathematics. CEACSE continued its efforts to broaden the scope of research through increased participation of additional faculty, graduate students and undergraduate students.

Highlights from this year's research include the work of Dr. Jin Wang, distinguished mathematician and UNUM Chair of Excellence in Applied Mathematics. Dr. Wang has been developing new solutions to model and simulate fluid-structure interactions with emphasis on energy efficiency applications. His foundational work is important to our research program development efforts in the Energy & Environment application area. The CEACSE funds for this project has resulted in two journal publications, one conference presentation, and two proposals for additional funding that are currently under consideration.

The work of Dr. Robert Webster is exemplary in demonstrating UTC's approach to engaging in strategic partnerships to bring experimentalists and computational engineers and scientists together to address important challenges. Dr. Webster has partnered with Purdue University to investigate efficient operations of turbo-machinery. The initial results of this project have been quite successful and resulted in one conference presentation and publication. The work is being carried over to FY17, which is likely to result in additional funding.

Dr. James Newman's work on the FUNSAFE (Fully UNStructured Adaptive Finite-Element) software system enables efficient execution of advanced PDE solvers using HPC hardware. This project extended the FUNSAFE program by adding a new capability to maintain consistent spatial discretization as the numerical solution of dynamical systems proceeds along the temporal dimension. This work has resulted in two additional publications and was awarded \$117,616 in additional funding by the Office of Naval Research. The project will continue to enable UTC researchers to react rapidly to new opportunities to attract extramural funding for new projects and programs.

Dr. Mina Sartipi's research has been particularly prolific this year. Her project entitled "Multi-modality Heterogeneous Data Analytics for Smart Health" developed a new framework for data pre-processing that allowed the development of a predictive analytics model for post-stroke recurrence. This work uses BigData to improve patient outcomes while reducing the cost of care. Combined with her project, "Sensing Communications and Analysis in SmartGrid," Dr. Sartipi has developed many community partnerships, produced 5 requests for external funding, and received \$119,829 from the NSF.

The table below lists the full activity of the CEACSE program for FY 16. (Financial information in Schedule 7 is attached in Appendix A)