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 2013-2014

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Executive Summary

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its ninth year of operation. The previous years have led to the establishment and development of an effective operation. During this entire time a culture of the securing external funding as an outcome of seed research funding provided by CEACSE has been fostered. There have been and continue to be some challenges as the Center continues operation. One issue is the necessity to promote and stimulate grant competition from a broader spectrum of individuals and technological areas. This is affected by current teaching demands, which impact capabilities and time required for research and proposal development and paths. There are continuing issues as well, the national economic environment, level of external monies committed to research and development funding, and increased externally competitive environment. The reporting year has proceeded with the awarded research funds being expended.

As is noted in this report, CEACSE continues to accomplish its mission and objectives. Through the awards, the researchers and associated academic units have maintained external funding from various agencies, companies, and governmental entities. CEACSE monies from the 2014 fiscal year as well as from past years continue to provide returns, reaping benefits through additional awards/grants. (Figure 1).

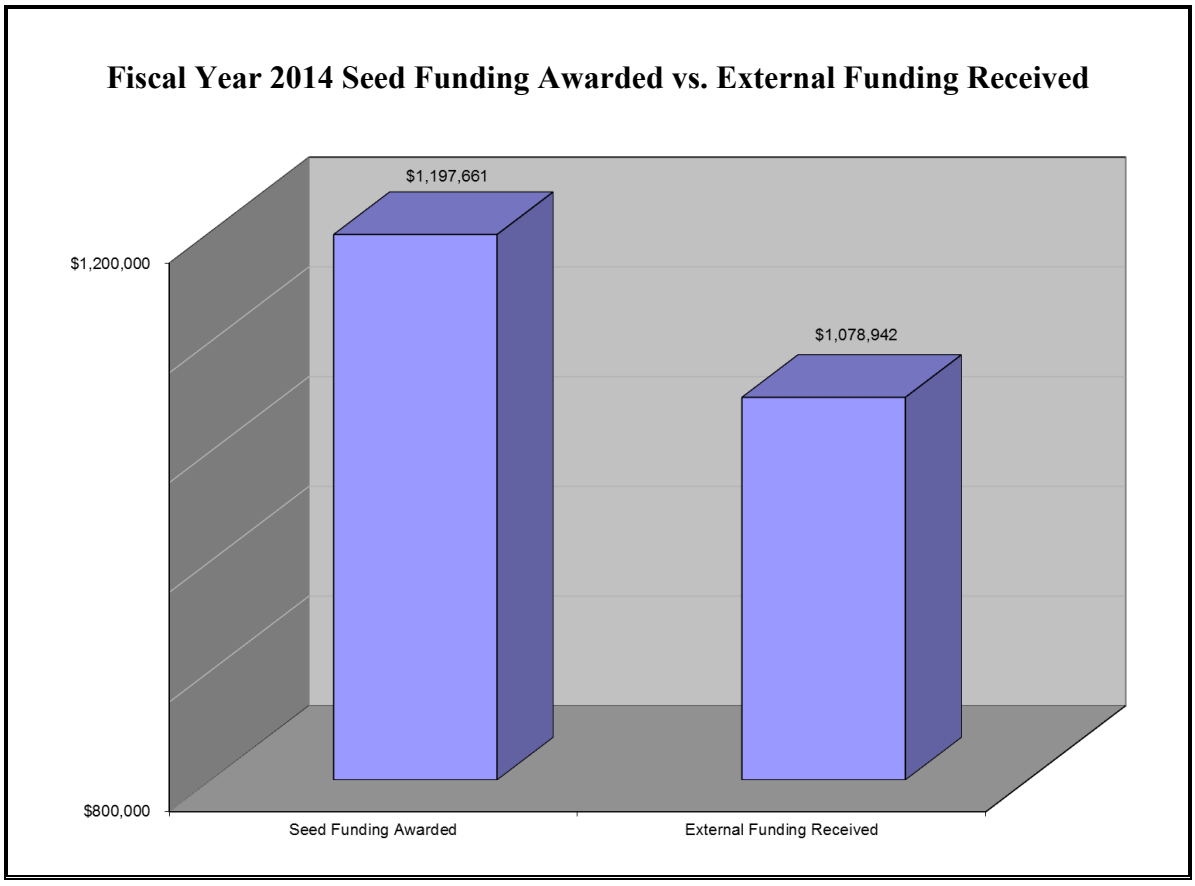

Figure 1

CEACSE continues to enhance the educational aspect of students through the Ph.D. and M.S. graduate programs at the University of Tennessee at Chattanooga and its Graduate School of Computational Engineering within the College of Engineering and Computer Science. There is a continuing reach to both graduate and undergraduate students and they have participated on various research activities undertaken as a result of CEACSE funding. Due to the research activities that some of the students have undertaken, local companies continue to have interest in the student's educational programs impacted by the CEACSE research. The SimCenter: National Center for Computational Engineering (SimCenter) continues to be a research anchor and attract students locally as well as nationally and internationally.

As noted in previous reports, an aspect of funding research activities and securing external funding assists in promoting companies to continue to develop offices here in the Chattanooga region.

The following is the Annual Report for Fiscal Year 2014 of CEACSE activities and efforts.

Introduction

Consistent with the enabling legislation which led to the formation of the THEC Centers of Excellence in 1984 et seq., the THEC Center of Excellence for Applied Computational Science and Engineering (CEACSE) presents opportunities to capitalize on the successful initiative of the SimCenter: National Center for Computational Engineering (SimCenter) and on the substantial transformational enabling investments made by a public/private community partnership. The vision for the original initiative was to recruit an established team of research, educational and professional staff members, who would form the SimCenter: National Center for Computational Engineering and the Graduate School of Computational Engineering within the College of Engineering and Computer Science at The University of Tennessee at Chattanooga. CEACSE builds upon the expertise to broaden and deepen the concept of a computational simulation center to consider a wider array of practical problem areas in science and engineering. This practice continues to seek and elicit additional faculty from across the University, particularly in areas of science and engineering, and has been based on the use of advanced computational methodologies to solve complex practical problems in applied science and engineering. The particular applications focus on interest areas to local and national industries and state and federal agencies. While funding from the Center seeds these activities, it anticipates that augmentation of the state funding would result from federal grants and contracts awarded to researchers for follow-on development in view of the expected wide interest in the resulting capability to solve problems of national interest.

This is the ninth year of operation of the UTC CEASCE and this report summarizes the research programs supported by CEASCE funds in FY2014 and the outcomes achieved by these programs in support of the Center of Excellence goals. Although the Center has been directed by Dr. Henry McDonald since its inception, Dr. McDonald retired at the end of July 2014. Upon his retirement, Dr. Neshlian Alp, Interim Dean of the College of Engineering and Computer Science at UTC, was appointed interim Director of CEASCE by UTC's Provost and Senior Vice Chancellor for Academic Affairs (Dr. Jerald Ainsworth). Dr. Alp will serve as Director of the Center until a permanent director is appointed.

Strategic Goal

The overarching goal of CEACSE is to be in accordance with the original enabling legislation and build upon the established UTC strength in applied computational science and engineering to evolve into and to be recognized as a national 'Center of Excellence' and a premier multidisciplinary research and education center for computational science and engineering. CEACSE utilizes the expertise and infrastructure of the existing SimCenter staff and its computing resources. CEACSE seeds new research activities, expands previously supported research activities, and undertakes supporting activities that lead to additional sources of funding. Appropriate faculty across the entire University and particularly those in science and engineering are encouraged and solicited to be involved. Thus, the research portfolio intends to broaden research contributions which enhance the educational and economic development mission of The University of Tennessee at Chattanooga.

Center Research Focus

CEACSE is strategically focused on synergistic new programs that will collectively advance the state of the art in computational simulation in solving complex problems in the physical sciences and engineering that require and utilize scientific supercomputing. This focus encompasses research on computational simulations for analysis of the physical processes embedded in real world problems in science and engineering, as well as computational approaches that synthesize these simulation capabilities into efficient and effective low-cost solution tools and capabilities across multiple disciplines. Complex problems in the physical sciences are frequently multidisciplinary and require a

synthesis of physical sciences, engineering, mathematics of computation, and scientific computing.

The Computational Approach

One of the major strengths of CEACSE is the SimCenter with its expertise in computational engineering and applications methodologies that are broadly applicable to both new and evolving problem areas and other non-engineering disciplines. CEACSE believes it is much easier and effective to encourage and develop teaming between professionals. These opportunities for experienced computational engineers to learn and adapt complex simulations in new physical disciplines by working with these experts without computational experience can create and accelerate new advancements and innovations. Seeded research activities both in new areas and in other disciplines involving the combination of experienced computational experts together with scientists who are expert in the required discipline, i.e. physics, chemistry, and biology, are sought and can be very effective in generating opportunities for research contributions and funding. This core computational expertise of the SimCenter is leveraged as necessary through interdisciplinary collaborations between SimCenter researchers who are experts in computational simulation, and collaborators who are experts in other disciplines or experts in a particular application area.

Objectives, Activities and Uses of Center Funding

The CEACSE pursues goals and objectives that establish the necessary and on-going foundation from which to develop and earn recognition as a premier center of excellence for computational applications in the physical sciences with national and international stature.

Objectives

The primary objective of the Center is to expand the demonstrated capability of the University in the area of Computational Science and Engineering and to seed research and educational activities that broaden and expand the Center's base of research expertise, thereby helping to attract new research funding.

The SimCenter has operational a significant cluster super computer. This machine is configured to perform and support computational simulations on large complex problems. Other organizations and universities around the world continue to upgrade their equipment, presenting continuing increased need for computing capability. This places increased pressure on existing resources for upgrading and/or defining access to other advanced computational capabilities that may be accessible. To achieve this access does require connection to advance communication and data networks to support such high level of data communication and security.

The utilization of available cluster-supercomputer resources for appropriate and promising research projects is of considerable importance. A ranking of a computing

machine is a measure of raw computing power, but does not necessarily directly correlate with the research undertaken or the results produced. CEACSE's philosophy is that the intellectual and practical value of each specific research project is the primary objective, and the computer itself serves as the enabling resource.

There has been an ongoing expansion of capabilities to broaden research and support activities. The Center requires that at least one external proposal be developed for each seed funded activity and submitted to a funding agency for continuation and expansion of the CEACSE funded research or related research. However, sometimes multiple years of funding are necessary to mature a technology, especially in emerging strategic focus areas. During this most recent year of operation it can be seen that the Center's funded activities and philosophies are continuing to achieve results (Table 1).

At the start of its ninth year, CEACSE granted funding to twenty-nine proposed research projects. In addition, several exploratory research activities were approved and funded during Fiscal Year 2014 (Table 2). The exploratory research activities included research performed in support of requests received from external funding agencies, efforts to find external funding opportunities for a number of the CEACSE funded projects, white paper and proposal preparation assistance, and research activities undertaken by the Center's Staff. As a result, several of these opportunities have been identified throughout the course of the fiscal year. The activities arise throughout the year and fall outside the standard award cycle. These exploratory

activities are evolving as increasingly important components of research activities. These are needed to respond increasingly to frequent demands to the new complex evolving problems. Consequently, these research activities were initiated at the discretion of the Center's Director based on needs and potential of following-on funding.

Table 1

CEACSE Seed Funding Committed for FY 2013-2014 Research Activities

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Development of Reduced Order Modeling Capabilities with Applications to Stability Derivative Evaluation and Computational Design	$35,000	Y	$28,278	N	N	
Numerical Simulation of Flow Structure Transport/Deposition of Particles in Pulmonary Airways	$35,000	Y	$30,160	Y	N	
Electromagnetic Simulations for Metamaterials and Frequency-Selective Surface	$60,000	Y	$44,316	N	N	
An Exploration of the Efficacy of HUGG Style Meshes on Turbo-Machinery	$25,000		$19,030	Y	Y	TVA, $10,000
Refactoring and Optimization of the Tenasi Tool Suite Code	$30,000	N	$8,030	N	N	
Quality of Service Assurance Using GENI	$45,000	Y	$27,258	N	N	
Numerical Simulation of Lithium-Ion Batteries	$20,000	Y	$18,334	N	N	
Molecular Dynamics Based Point Generation and Radical Basis Flow Solver	$35,000	Y	$33,237	Y	Y	ONR, $296,317
High-Order Space-Time Approach	$40,000	N	$39,857	N	N	
Technology Development for Multiphysics Simulation, Sensitivity and Design	$40,000	Y	$29,886	Y	Under Review	ONR, $990,000 (under review)
Transition Modeling for Improved Heat Transfer Computations for Turbomachinery	$20,000	Y	$18,749	N	N	
Incompressible Multi-Species Flow Regime with Total Energy Conservation	$30,000	Y	$26,496	Y	Y	CHI Engineering, $47,878
Design of a Coronary Stent for Reduced Failure Rates	$10,000	Y	$8,611	Y	N	
Validation and Application of the Tenasi Particle Module	$35,000	Y	$30,823	Y	N	
Rapid Generation of Animations from Tenasi Simulations	$16,957	Y	$13848	N	N	
Communication and Data Processing Tools for Automated Fall Risk Assessment System	$35,000	Y	$17,008	Y	Y	NIH, $384,747
Data Acquisition and communication in Smart Grid Networks	$35,000	Y	$21,933	N	N	
High-Order Methods for the Compressible Navier-Stokes Equations	$50,000	Y	$36,590	Y	Y	High Performance Technologies, $120,000
Aero-Elastic Study of the Turbofan Stage for the Energy Efficient Engine	$50,000	Y	$41,639	N	N	
Validation Simulations of the Turbofan and Boost Stages of the Energy Efficient Engine	$10,000	Y	$8,315	N	N	
Solver Enhancements for Simulation of Objects in Dynamic Contact Using Combined Immersed Boundary and Overset Grid Methods	$20,000	Y	$17,505	Y	Y	ONR, $220,000

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Development of a Fully-Coupled Fluid Structure Interaction Approach for Hydrodynamic Applications	$40,000	Y	$36,343	N	N	
Arbitrary Lagragian-Eulerian Method for Blast Simulations	$40,000	Y	$38,503	N	N	
Bioinformatics Analysis of Human Genes Associated with Diseases at Higher Rates in African Americans DHRAAs	$60,000	N	$65,397	Y	N	
Zero-Based Knowledge Authentication in Aerial Networks	$5,000	Y	$3,996	N	N	
Undergraduate Research Assistantship Program in Computational Science and Engineering	$5,000	N	$5,000	N	N	
Stent Design Proposal Preparation	$10,000	N	$10,000	N	N	
TOTAL	**$836,957**		**$772,310**			

Table 2

CEACSE Seed Funding Carried Forward from FY 2012-2013 to FY 2013-2014 Research Activities

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
A Power Efficient Multicasting Scheme Using Compressive Sensing	$51,660	N	$38,927	N		
Authentication in Mobile Platforms	$54,244	Y	$54,241	N		
TOTAL	**$105,904**		**$93,168**			

Table 3

CEACSE Exploratory Research Activities for FY 2013-2014

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Investigation of Alternative Boundary Condition Formulations	$5,581	N	$5,581	N	N	
Adjoint Equation Convergence Enhancement	$2,191	N	$2,191	N	N	
Performance Improvement of Grid Generation Software	$3,477	N	$3,477	N	N	
Automation of the Generation of Overset Grids	$7,085	N	$7,085	N	N	
Survey of Current State of the Art for Hypersonic Applications	$3,417	N	$3,417	N	N	
Post Processing Enhancements for Multiphase Flows	$4,804	N	$4,804	N	N	
Streamlined Workflow Component Integration	$4,704	N	$4,704	N	N	
Investigation of WENO Schemes in Tenasi	$1,374	N	$1,374	N	N	
Improvements in Stall Prediction	$1,123	N	$1,123	N	N	
Increasing Robustness of Overset Grid Approaches	$2,679	N	$2,679	N	N	
TOTAL	**$36,436**		**$36,434**			

Table 4

Summary of Funds Budgeted and Expended for FY 2013-2014

Expense	Budget	Expenses
SimCenter R&D Support	$149,541	$149,541
CEACSE Seed Funding for FY 2012-2013 Projects	$836,957	$772,310
CEACSE Seed Funding for FY 2011-2012 Projects Carried Forward	$105,904	$93,168
CEACSE Exploratory Research Activities	$36,434	$36,434
TOTAL	**$1,128,836**	**$1,051,453**

In order to ensure that the objectives of the Center's investment continue to be met, the financial progress of the projects is routinely tracked on a monthly basis via the UT financial reporting system, and the technical progress of the projects is monitored via short monthly progress reports, and final reports submitted to the Center by the Principal Investigators. Subsequent external funding is also tracked and where appropriate is attributed to a specific Center project or groups of projects. Recipients of CEACSE seed funding are required to provide a copy of their submitted proposal and any subsequent information regarding award or non-award of follow on external funding.

A secondary objective is to increase the participation of additional faculty, graduate and undergraduate students in the Center's research efforts and where possible assist in the recruitment of new faculty and students to the University.

CEACSE continued its efforts to broaden the scope of research through increased participation of additional faculty, graduate students and undergraduate students. CEACSE awarded seed funding to support the research activities of 18 faculty members from various disciplines, such as physics, computer science, and computational engineering.

Another objective is to engage in activities that are directly or indirectly supportive of economic development initiatives that benefit Tennessee, in particular activities that

create collateral opportunities for new research.

The Center has had numerous visitors to discuss opportunities for research collaboration, and the Center has given numerous presentations at meetings hosted at the SimCenter on the UTC campus. During the past nine years, CEACSE faculty have made numerous presentations during meetings for discussions directly related to metropolitan engagement for the purpose of economic development, support of local businesses and government, and planning for SimCenter expansion. Some notable discussions, pertaining to research opportunities, occurred during this report period with Performance Innovation Transport, CHI Engineering, and TVA. Research issues discussed included effectiveness of Class 8 vehicle aerodynamic drag reduction devices, containment of liquefied natural gas spills, and light-water nuclear reactor simulations. In addition, CEACSE sponsored research has created numerous opportunities for education of graduate students, thereby providing students the potential to secure high-paying quality positions and to be able to remain within Tennessee. Finally, CEACSE sponsored research contributes to and enables the following activities at the SimCenter that are supportive of economic development:

1. SimCenter personnel have recently held discussions with Yves Procvencher of Performance Innovation Transport (PIT), a non-profit company based in Quebec (Canada). This company is performing testing and analysis on behalf of a consortium made up of over 50 trucking fleets across Canada (and two from the U.S.). The discussions are very preliminary and are currently

focused on determining how the SimCenter's expertise in physics-based computational simulation can add value to PIT's use of physical testing for determining the performance of various products designed to enhance efficiencies of large Class 8 trucks, including aerodynamic devices. The current plan is to team with our ORNL colleagues as well as PIT and then approach both U.S. and Canadian government agencies (e.g., EPA from the U.S.) for funding to pursue a "clearing house" Center which could address the performance-enhancement needs of trucking fleets across North America. Two U.S. drag reduction device manufacturers, SmartTruck Systems (STS) and Advanced Transit Dynamics (ATD), are already taking advantage of the SimCenter's expertise in computationally evaluating device performance.

2. The SimCenter was contracted by CHI Engineering to simulate a catastrophic failure of a liquefied natural gas (LNG) containment vessel for one of CHI Engineering's clients. These containment vessels are quite large (~120ft tall and ~150 ft in diameter), and a complete failure of the containment vessel will release a substantial amount of LNG, which will eventually vaporize into the atmosphere and pose a significant fire hazard if the cloud is ignited. LNG containment vessels are typically surrounded by berms that will hold any spill near the storage facility and prevent the LNG from flowing into adjacent areas in order to minimize any fire hazard. CHI Engineering's client is concerned that although the berms surround an area large enough to contain the LNG sitting at rest, the berms may not be high enough to prevent the wall of

flowing LNG from overtopping them and escaping the holding pond while traveling at high speed after a complete failure of the LNG containment vessel. The SimCenter will evaluate two existing LNG sites to determine if additional retaining walls and/or height modifications to the existing berms need to be utilized to prevent the flowing LNG from escaping the holding pond.

3. TVA has approached the SimCenter in regards to simulation of light-water nuclear reactors. This work is being done as part of the CASL project (Consortium for Advanced Simulation of Light-Water Reactors) through TVA and is concerned with grid generation issues associated with a complete reactor vessel. The present work, however, is focused on gridding a smaller region called the "lower plenum chamber" which contains considerable support structures and, as such, can adversely affect the flow of cooling water through this region of the reactor vessel. The TVA project coordinator is confident that the SimCenter can become a grid generation resource for the Consortium and thereby attract more substantial resources commensurate with gridding needs.

A final objective is to seek appropriate opportunities for educational outreach activities that a) help to create awareness and to stimulate interest in science and engineering among pre-college students, and b) help to stimulate interest in graduate study at UTC among undergraduate and graduate students.

STEM School Chattanooga students visited the SimCenter twice in the spring of 2014 as part of a unit they were teaching that included computer simulation. The students were divided into teams and asked to write Python code to simulate some aspect of a nuclear attack on California. The team leaders and school Principal visited the SimCenter where SimCenter faculty and staff provided instruction about computer simulation. The students also toured the SimCenter and learned about the high-performance computing abilities of the center. Later in the spring, the school selected a smaller set of students to return to the SimCenter to present their work. Scalability testing was performed on one of the team's code using the SimCenter's fastest cluster.

Forty seven rising high school juniors and seniors (plus six faculty and staff) from Austin Peay State University's (APSU) Governor's School for Computational Physics visited the SimCenter on June 6. This was their eighth year of visiting the SimCenter and UTC. The Governor's School founding director, Dr. Jaime Taylor (now interim Provost at APSU) was also with the group and stated that "We've visited the SimCenter now for several years and this trip is always one of the students' favorites, and that's saying something because they also visit Marshall Space Flight Center and NICS at ORNL."

In mid-January Ms. Lindsey Cleary resigned from her position as the SimCenter's STEM Coordinator to accept a position with Mozilla. Although Mozilla is a California-based company, Lindsey will continue to work and live here in Chattanooga. Mozilla is expanding its presence in Chattanooga and Lindsey was asked to lead the effort associated with this expansion. Lindsey has been an extremely valuable asset to the SimCenter and made significant strides in expanding the SimCenter's STEM presence in the City and surrounding region. We certainly wish her all the best in her new adventure with Mozilla. Since Lindsey's departure, the SimCenter's STEM-related activities have necessarily been reduced. However, we try very hard to host as many groups as is practical involving faculty and students who have been involved in these activities. At present, there are no plans to replace Lindsey due to budgetary concerns.

Center Plan for Achieving Objectives

The operation of the Center is guided by strategic planning to identify promising research avenues within the broad area of applied computational science and engineering. Some promising areas have been identified that leverage existing research capabilities into new and related areas. The Center continues to seek ongoing participation from other UTC faculty and personnel to identify additional areas of strength based on their individual expertise and synergism with other Center activities. The Center continues to solicit these activities through a campus wide request for white papers and proposals. These white papers briefly describe the proposed effort, anticipated results, support required and a potential source of continued research funding, e.g. target agency, request for proposal

etc. The Center provides seed funding for initiatives in the most promising areas for project and program planning aimed at developing competitive proposals for new external funding. Such seed funding includes faculty and student support for exploratory feasibility studies, demonstration of new capability supporting proposals, contacts with sponsoring agencies, proposal development, and related travel. This solicitation procedure is a part of CEACSE annual operating cycle.

The criteria for evaluating promising research areas and initiatives includes relevance and potential for contributing to success in becoming an accomplished Center of Excellence through the Center's goals of a) sustainable growth in research funding, b) excellence in integrated research and education, c) increase in national and international stature, and d) promoting regional economic development and economic competitiveness for the State of Tennessee.

Research Activities Funded by the Center

The following list of activities and uses of funding illustrate how the Center's plan has begun to establish Center cohesion and synergism that fosters innovation and fills gaps that would otherwise arise from multiple individual research grants that are driven by the diverse and shorter term needs of the sponsoring agencies. (Schedule 7 is attached)

Extended Research Activities Funded by the Center in Fiscal Year 2011-2012 and Continued in Fiscal Year 2013-2014

1. **Authentication in Mobile Platforms**
    - Principal Investigator(s): Dr. Li Yang, Computer Science and Engineering Objective(s): Investigate current status and challenges of securing mobile devices; Innovate cryptographic algorithms and protocols to authenticate both mobile devices and mobile users; Secure communication between mobile devices to remote or a cloud; Propose and implement solution to management identity of mobile users together with access control to a remote cloud.
    - Seed Funding: $54,244
    - Results: Technology still being developed.

2. **A Power Efficient Multicasting Scheme Using Compressive Sensing**
    - Principal Investigator(s): Dr. Mina Sartipi, Computer Science and Engineering
    - Objective(s): To develop a distributed multihop multicast scheme that is simple, energy efficient, and reliable.
    - Seed Funding: $51,660
    - Results: Technology still being developed.

New Research Activities Funded by the Center in Fiscal Year 2013-2014

1. **Development of Reduced Order Modeling Capabilities with Applications to Stability Derivative Evaluation and Computational Design**
    - Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
    - Objective(s): To assess the feasibility, efficiency, and accuracy of developing complimentary sensitivity-based unsteady aerodynamic ROMs.
    - Seed Funding: $35,000
    - Results: More time is needed to explore this interdisciplinary topic and apply it to aerospace engineering applications.

2. **Numerical Simulation of Flow Structure and Transport/Deposition of Particles in Pulmonary Airways**
    - Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
    - Objective(s): The primary focus of this work was time dependent boundary conditions for both inflow/outflow boundaries and viscous boundaries.
    - Seed Funding: $35,000

- Results: Proposal submitted to NSF for $295,208 which was not selected for funding.

3. **Electromagnetic Simulations for Metamaterials and Frequency-Selective Surface**
    - Principal Investigator(s): Dr. Kyle Anderson, Graduate School of Computational Engineering
    - Objective(s): Incorporate the frequency-dependent materials into the 3D code; Generalize port I/O to greatly extend the applicability of the code; Modify the linear algebra routines to accommodate solving for a different number of unknowns in various regions; Validation for frequency-selective surfaces, metamaterials, and frequency-dependent materials.
    - Seed Funding: $60,000
    - Results: Frequency-dependent materials have been implemented and the other modifications to the 3D code are complete. Modifications for metamaterials are under way and preliminary results have been obtained.

4. **An Exploration of the Efficacy of HUGG Style Meshes on Turbo-Machinery**
    - Principal Investigator(s): Mr. C. Bruce Hilbert, Graduate School of Computational Engineering
    - Objective(s): To show that MBHUGG meshes will capture relevant flow features as well as traditional structured grids while allowing for many of the advantages of unstructured grids.
    - Seed Funding: $25,000
    - Results: Proposal Submitted to TVA for $10,000 and funded.

5. **Refactoring and Optimization of the Tenasi Tool Suite Code**
    - Principal Investigator(s): Dr. Daniel Hyams, Graduate School of Computational Engineering
    - Objective(s): To refactor and reengineer the Tenasi Code in order to make it more accessible for researchers and potential customers. In addition, the refactoring and optimization will better position Tenasi for petascale to exascale computations.
    - Seed Funding: $30,000
    - Results: Faculty member left the university so only a portion of the envisioned refactoring was completed.

6. **Quality of Service Assurance using GENI**
    - Principal Investigator(s): Dr. Farah Kandah, Computer Science and Engineering
    - Objective(s): To address the challenges that could degrade the network performance, thus degrading its quality of service, where new practical and theoretical approaches will be provided taking into consideration the delay and the throughput optimization.

- Seed Funding: $45,000
- Results: Technology is still being developed.

7. Numerical Simulation of Lithium-Ion Batteries

- Principal Investigator(s): Dr. Sagar Kapadia, Graduate School of Computational Engineering
- Objective(s): To develop a three-dimensional simulation capability for analysis of Lithium-Ion batteries with particular emphasis on temperature modeling within the battery.
- Seed Funding: $20,000
- Results: A three-dimensional Li-Ion battery model was developed under the THEC grant. During recent discussion with Oak Ridge National Laboratory researchers, numerical simulation of Lithium-Ion batteries was identified as one of the research topics for collaboration. In the future, potential collaboration opportunities with ORNL will be explored for external grants.

8. Molecular Dynamics-Based Point Generation and Radial Basis Flow Solver

- Principal Investigator(s): Dr. Steve Karman, Graduate School of Computational Engineering
- Objective(s): Develop molecular-dynamics based point cloud generator for 3D; Develop radial-basis based Euler solver for flow field simulation; Combine the point generation and Euler solver in a dynamic case with body motion
- Seed Funding: $35,000
- Results: Proposal submitted to ONR for $296,317 and funded.

9. High-Order Space-Time Approach

- Principal Investigator(s): Dr. Lafayette Taylor, Graduate School of Computational Engineering
- Objective(s): To extend the Navier-Stokes solver to three-dimensions, perform validation cases, and determine the efficiency margin.
- Seed Funding: $40,000
- Results: Preliminary results obtained for simple geometries and a novel method was conceived for complex geometries which will be developed through a new THEC project.

10. Technology Development for Multiphysics Simulation, Sensitivity, and Design

- Principal Investigator(s): Dr. James C. Newman, Graduate School of Computational Engineering
- Objective(s): To extend the element formulations within the structural analysis component of FUNSAFE; To develop consistent sensitivity

analysis technology within the structural analysis solver to enable multidisciplinary sensitivity analysis and design optimization, and to develop a basic overlapped grid capability for higher-order finite element discretizations.

- Seed Funding: $40,000
- Results: A higher-order streamline/upwind Petrov-Galerkin overset grid scheme was developed for moving domains. The methodology was validated using the method of manufactured solutions for linear, quadratic, and cubic elements. Additionally this technology was demonstrated for large relative motion between multiple, interacting bodies. An unsolicited joint proposal with UTC (lead), Massachusetts Institute of Technology (MIT), and the Naval Surface Ware Center Carderock Division (NSWCCD) was submitted to the Office of Naval Research. The proposal leverages the capabilities developed and results obtained through this THEC funding. The initial estimated three year budget is $990K.

11. Transition Modeling for Improved Heat Transfer Computations for Turbomachinery

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering
- Objective(s): A correlation-based transition model that is dependent on local variables will be implemented into Tenasi; Establish the framework to apply the transition terms to all of the turbulence models in Tenasi; Identify test cases and validate the transition model for turbomachinery applications.
- Seed Funding: $20,000
- Results: Future work will focus on evaluating the Langtry model on various test cases and upon extending the transition model to additional turbulence models in Tenasi.

12. Incompressible Multi-Species Flow Regime with Total Energy Conservation

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering
- Objective(s): Evaluate multiple models to identify the model that offers the greatest extension to Tenasi; Extend the thermal equation to conserve total energy; Implement the Incompressible Multi-Species model into Tenasi; Establish the framework for activating specific functionality such as humidity or chemical reactions; Identify test cases and validate the new flow regime.
- Seed Funding: $30,000
- Results: Proposal submitted to CHI Engineering for $47,878 and funded.

13. Design of a Coronary Stent for Reduced Failure Rates

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering
- Objective(s): To employ CFD and optimization techniques to design streamlined wire cross-sectional shapes that maintain WSS levels above an minimum level.
- Seed Funding: $10,000
- Results: A proposal was submitted to NIH and was not successful.

14. Validation and Application of the Tenasi Particle Module

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To validate the Tenasi particle module for a wide variety of fluid flows laden with particulate matter such as airborne viruses, inhalants and environmental PM10. The validation areas will correspond to application areas such as mitigation of airborne biological contaminants, improved inhalant design and PM10/PM2.5 mitigation in the urban environment.
- Seed Funding: $35,000
- Results: Proposal was submitted to NSF and was not selected for funding.

15. Communication and Data processing Tools for Automated Fall Risk Assessment System

- Principal Investigator(s): Dr. Mina Sartipi, Computer Science & Engineering
- Objective(s): To study the data communication and data analysis required for automated estimation of fall risk for post stroke patients.
- Seed Funding: $35,000
- Results: Proposal was submitted to NIH for $384,747 and awarded.

16. Data Acquisition and Communication in Smart Grid Networks

- Principal Investigator(s): Dr. Mina Sartipi, Computer Science & Engineering
- Objective(s): Proposing a data communication for the power transmission/generation premise; Providing an uninterrupted communication link for cellphone coverage during disaster relief. This will provide and alternative solution to using the existing emergency channels allocated to emergency services.
- Seed Funding: $35,000
- Results: Technology is still being developed. This project was extended through FY15.

17. High-Order Methods for the Compressible Navier-Stokes Equations

- Principal Investigator(s): Drs. Li Wang and Kyle Anderson, Graduate School of Computational Engineering
- Objective(s): To continue the development of higher-order accurate discontinuous Galerkin (DG) and Petrov-Galerkin (PG) methods for delivering high-accuracy solutions of the Navier-Stokes equations.
- Seed Funding: $50,000
- Results: Proposal submitted to High Performance Technologies for $120,000 and funded.

18. Aero-elastic Study of the Turbofan Stage for the Energy Efficient Engine

- Principal Investigator(s): Dr. Robert Webster, Graduate School of Computational Engineering
- Objective(s): Conduct simulations without modal analysis to compare against measured aerodynamic performance; Conduct simulations with modal analysis included to compare against the measured blade dynamic and aerodynamic performance; Examine details of flow field to gain better understanding of the physics of the problem.
- Seed Funding: $50,000
- Results: Due to the complex nature of the turbofan stage, both from a geometrical and flow physics standpoint, algorithmic parameters and sensitivities were investigated prior to performing the actual aero-elastic analysis. Meeting with other universities concerning this work have taken place to investigate the possibility of collaborating on proposals to private industries and NASA.

19. Validation Simulations of the Turbofan and Boost Stages of the Energy Efficient Engine

- Principal Investigator(s): Dr. Robert Webster, Graduate School of Computational Engineering
- Objective(s): Conduct simulations based on smallest possible axisymmetric sector for original blade/vane counts of fan, outlet guide vanes, rotor and stator of boost compressor at matched bypass ratio and operating speeds; compare with experiment
- Seed Funding: $10,000
- Results: It is planned in the near future to discuss possibilities with personnel at NASA-Glenn Research Center; it is also planned to explore possibilities of collaborative research with faculty at Purdue University, who are engaged in experimental turbomachinery work.

20. Solver Enhancements for Simulation of Objects in Dynamic Contact Using Combined Immersed Boundary and Overset Grid Methods

- Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): To leverage recent progress in the implementation of immersed boundary and overset grid capabilities to simulate flow fields for objects with intermittent dynamic contact.
- Seed Funding: $20,000
- Results: Proposal submitted to ONR for $220,000 and funded.

21. Development of a Fully-Coupled Fluid Structure Interaction Approach for Hydrodynamic Applications.

- Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): To leverage past research on hydrodynamic applications and recent progress in the development of an in-house fluid structure interaction capability for the Tenasi flow solver.
- Seed Funding: $40,000
- Results: Implementation and testing of this approach into the Tenasi solver was started under this research. Some additional work is needed to complete this testing and debugging process and to demonstrate that this method is feasible for large scale deformations of practical ship hulls.

22. Arbitrary Lagragian-Eulerian Method for Blast Simulations

- Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): The development and implementation of an arbitrary Lagragian-Eulerian method in the Tenasi flow solver.
- Seed Funding: $40,000
- Results: Several key component technologies for the ALE formulation were implemented, tested and demonstrated. Development of the final components is needed to obtain preliminary results to include in proposals.

23. Bioinformatics Analysis of Human Genes Associated with Diseases at Higher Rates in African Americans

- Principal Investigator(s): Dr. Li Yang, Computer Science and Engineering
- Objective(s): Perform large-scale computational searches to identify candidate human genes that are under recent-selection in African and African derived populations; Evaluate pathogenic significance of genes under recent selections based on gene networks.
- Seed Funding: $60,000
- Results: Proposal for $190,590 submitted to NSF and declined; Proposal submitted for $119,878 submitted to NSF and declined; Proposal in the amount of $425,035 submitted to NSF and declined.

24. Zero-based Knowledge Authentication in Aerial Networks

- Principal Investigator(s): Ms. Katherine Winters, Computer Science and Engineering
- Objective(s): To build a preliminary protocol for use in zero-based knowledge aerial authentication
- Seed Funding: $5,000
- Results: Technology still being developed.

25. Undergraduate Research Assistantship Program in Computational Science and Engineering

- Principal Investigator(s): Dr. Louie Elliot, College of Engineering
- Objective(s): To establish an Undergraduate Research Assistantship program in Computational Science and Engineering for students at the University of Tennessee at Chattanooga.
- Seed Funding: $5,000
- Results: Five undergraduate research assistants were funded for the Fall 2013 semester.

26. Stent Design Proposal Preparation

- Principal Investigator(s): Dr. Robert Melnik, Graduate School of Computational Engineering
- Objective(s): To develop and submit a stent proposal to NIH
- Seed Funding: $10,000
- Results: A proposal was submitted to NIH and was not selected for funding.

27. Rapid Generation of Animations from Tenasi Simulations

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To develop a tool that can generate animations of transient Tenasi simulations with minimal user effort.
- Seed Funding: $16,957
- Results: Technology developed and ready to use.

Summary of CEACSE funding allocation (Figure 2) illustrates the major categories into which the CEACSE budget was allocated for Center activities during the past fiscal year of operation. It should be noted that grant awards from proposals and funding requests sought from this fiscal year funded projects normally will lag 6 to 12 months.

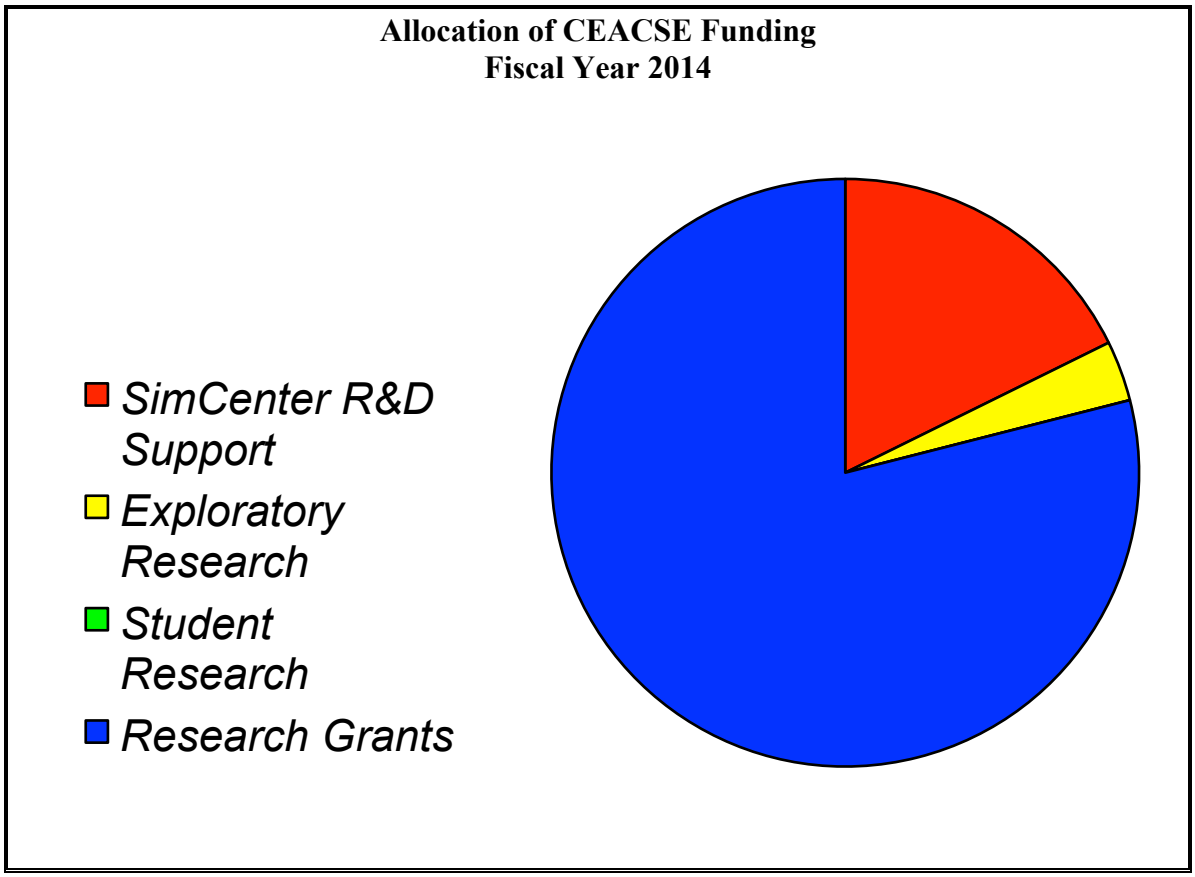

Figure 2

External Funding Awarded as the Result of the Center's `Research Investment*

External Funding Awarded in Fiscal Year 2005-2006:	$ 2,195,529
External Funding Awarded in Fiscal Year 2006-2007:	$ 3,291,102
External Funding Awarded in Fiscal Year 2007-2008:	$ 1,855,276
External Funding Awarded in Fiscal Year 2008-2009:	$ 4,765,948
External Funding Awarded in Fiscal Year 2009-2010:	$ 6,427,956
External Funding Awarded in Fiscal Year 2010-2011:	$ 1,111,097
External Funding Awarded in Fiscal Year 2011-2012:	$ 1,125,837
External Funding Awarded in Fiscal Year 2012-2013	$ 1,853,443
External Funding Awarded in Fiscal Year 2013-2014	$ 1,078,942
Total External Funding Awarded:	**$23,705,130**

* These funds represent funds committed by external funding agencies. Some of the awards included are multi-year awards with each year's funding dependent upon availability of funds.

A multi-year view of the outcomes achieved by CEACSE is portrayed in Figure 3. The outcome from funding provided to CEACSE by The State of Tennessee and The University of Tennessee at Chattanooga illustrates the achievement of a two-to-one ratio when compared to the amount of external funding generated by the State's investment in research. As illustrated, this rate of return continues through FY14. This performance has been consistent and CEACSE works toward continuous improvement.

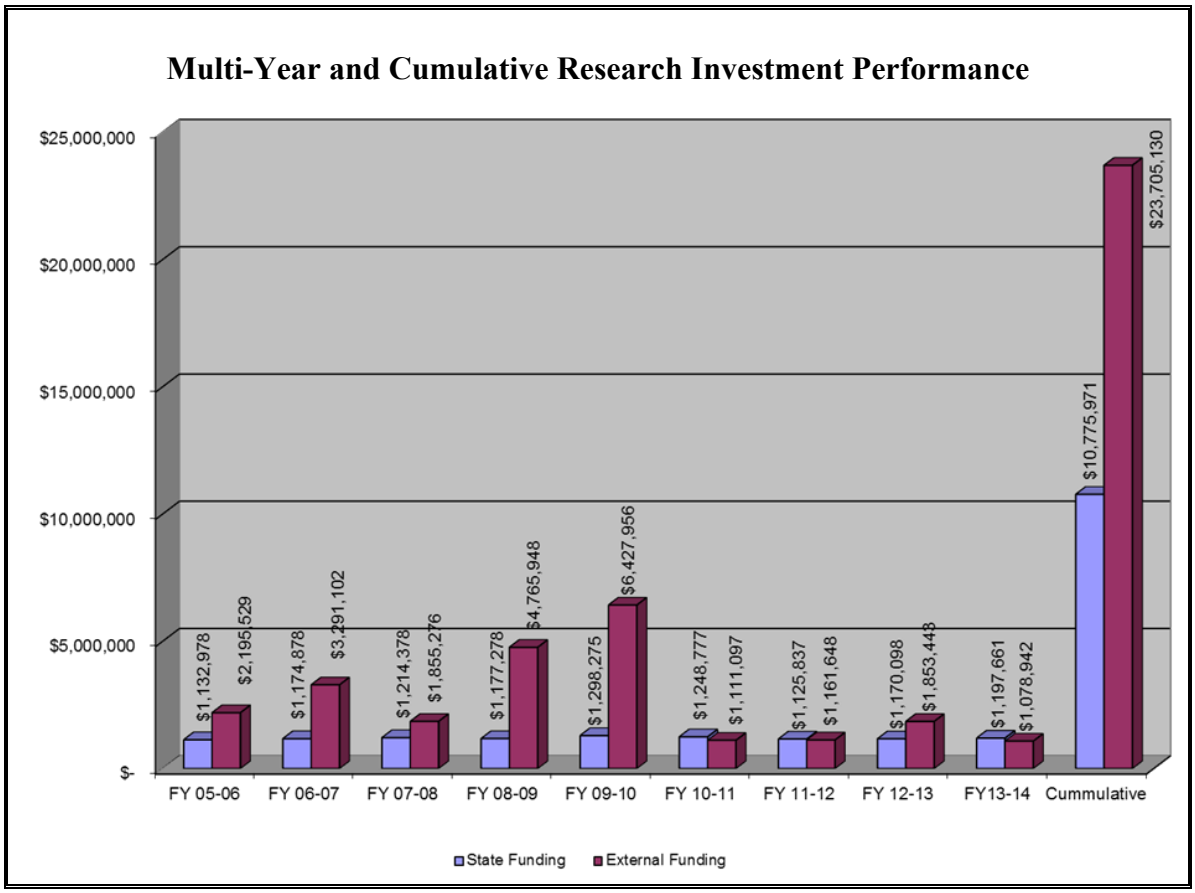

Figure 3

FY 2014 Publications and Presentations of the Center's Research Activities

1. Ahrabi, B.R., Anderson, W.K., Newman III, J.C., "High-Order Finite-Element Method and Dynamic Adaptation for Two-Dimensional Laminar and Turbulent Navier-Stokes," 32nd AIAA Applied Aerodynamics Conference, June 2014, AIAA Paper 2014-2983.
2. Liu, C., Newman III, J.C., Anderson, W.K., "A Streamline/Upwind Petrov Galerkin Overset Grid Scheme for the Navier-Stokes Equations with Moving Domains," 32nd AIAA Applied Aerodynamics Conference, June 2014, AIAA Paper 2014-2980.
3. Wang, L., Anderson, W.K., Erwin, T. and Kapadia, S., "Discontinuous Galerkin and Petrov Galerkin Methods for Compressible Viscous Flows," Computers and Fluids, Vol. 100, pp. 13-29.
4. Wang, L., Anderson, W.K., Kapadia, S. and Taylor, L.K., "Multiscale Large Eddy Simulation of Turbulence Using High-Order Finite Element Methods," 7th AIAA Theoretical Fluids Mechanics Conference, Atlanta, GA, June 2014, AIAA Paper 2014-3211.
5. Sreenivas, K., Mittal, A., Hereth, L., Taylor, L.K., and Hilbert, C.B., "High-Fidelity Computational Simulation of the Interaction between Tandem Wind Turbines," 32nd AIAA Applied Aerodynamics Conference, June 2014, AIAA Paper 2014-2278.
6. Mittal, A., Sreenivas, K., Taylor, L.K., Hereth, L., Hilbert, C.B., and Hyams, D.G., "Investigation of Rotor Models for Wind Turbine Simulations," 32nd AIAA Applied Aerodynamics Conference, Atlanta, GA, June 2014, AIAA Paper 2014-2280.
7. Gupta, A., Sreenivas, K., and Taylor, L.K., "Preconditioning Methods for Multiphase Flows," 11th AIAA/ASME Joint Thermophysics and Heat Transfer Conference, Atlanta, GA, June 2014, AIAA Paper 2014-2824.
8. Currier, N., and Sreenivas, K., "A Preconditioned Non-Singular Eigensystem for the Navier-Stokes Equations with Finite-Rate Chemistry," 7th AIAA Theoretical Fluids Mechanics Conference, Atlanta, GA, June 2013, AIAA Paper 2014-3084.
9. Mittal, A., Sreenivas, K., and Taylor, L.K., "Exploration of Modal Decomposition Techniques for Wind Turbines," AIAA-2014-1398, SciTech 2014, National Harbor, MD, January 2014.
10. Karman, S. L., "Multi-Block Hierarchical Unstructured Grid Generation With Adaptation," AIAA-2014-0116, SciTech 2014, National Harbor, MD, January 2014.
11. Currier, N., Franko, K., "A Discrete Error Transport Equation Source Model for Mesh Adaptation," AIAA-2014-1431, 52nd AIAA Aerospace Sciences Meeting, National Harbor, MD, January 2014.

Conclusion

CEACSE has established operations and is positioned to continue to enhance and expand research and assist in the obtaining of external funding opportunities. Research funding for a number of diverse projects has engaged more faculty and students across the campus. The committed seed funding enabled various faculty to pursue their research and develop opportunities to obtain follow-on support externally. The Center has a requirement for recipients of funding to submit proposals to a credible agency and/or company which have an interest in the research being conducted. As evidenced, there is already a growing level of external funding being sought from the activities of the Center. This should continue. With current external economic conditions and funding levels for research, there is increased competitiveness for the available funding. The SimCenter continues to be competitive and is increasing efforts to remain a highly viable competitor to secure funding.

There have been increased activities in both direct and indirect support of economic development for Tennessee. There have been a number of meetings with local and regional companies as well as indirect impacts. It is anticipated that these activities will continue.

Through the seed funding for research activities, undergraduate and graduate students are being engaged in a diverse range of topics. Additional efforts in this area assist in increasing the interaction and involvement of students with research faculty. Additional

efforts will need to be defined, focused, and initiated to enhance/increase outreach to pre-college students. This area will receive additional and continued attention.

Finally, the role engineering and science must take in the US and Tennessee to maintain and improve our economy is increasingly apparent. CEACSE is emphasizing and supporting the leveraging of its funding to enhance Tennessee's stature in engineering, science, and education in the arena of computational science and engineering. This in turn contributes to the ongoing economic development of Tennessee and the Chattanooga area. CEACSE believes if additional funding can be identified for CEACSE, it would be possible for the Center to leverage, enhance and accelerate this growth and advancement of Tennessee's scientific and engineering capabilities and resources.

Schedule 7

CENTERS OF EXCELLENCE/CENTERS OF EMPHASIS
ACTUAL, PROPOSED, AND REQUESTED BUDGET

Institution UTC **Center** Center of Excellence in Applied Computational Science & Engineering

	FY 2013-14 Actual			FY 2014-15 Proposed			FY 2015-16 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures	405,600	792,061	**1,197,661**	405,600	773,015	**1,178,615**	405,600	811,666	**1,217,266**
Salaries									
Faculty	185,873	360,813	**546,686**	280,000	520,000	**800,000**	222,750	452,250	**675,000**
Other Professional	22,762	44,186	**66,948**	35,000	65,000	**100,000**	24,750	50,250	**75,000**
Clerical/ Supporting	0	0	**0**	0	0	**0**	0	0	**0**
Assistantships	21,117	40,992	**62,110**	70,000	130,000	**200,000**	36,300	73,700	**110,000**
Total Salaries	**229,753**	**445,991**	**675,744**	**385,000**	**715,000**	**1,100,000**	**283,800**	**576,200**	**860,000**
Longevity	**435**	**845**	**1,280**	**700**	**1,300**	**2,000**	**660**	**1,340**	**2,000**
Fringe Benefits	58,061	112,706	**170,767**	98,000	182,000	**280,000**	70,950	144,050	**215,000**
Total Personnel	**288,249**	**559,542**	**847,791**	**483,700**	**898,300**	**1,382,000**	**355,410**	**721,590**	**1,077,000**
Non-Personnel									
Travel	3,456	6,708	**10,164**	10,500	19,500	**30,000**	9,900	20,100	**30,000**
Software	0	0	**0**	5,250	9,750	**15,000**	4,950	10,050	**15,000**
Books & Journals	0	0	**0**	4,150	1,871	**6,021**	6,795	1,971	**8,766**
Other Supplies	2,038	3,956	**5,994**	7,000	13,000	**20,000**	6,600	13,400	**20,000**
Equipment	1,105	2,144	**3,249**	3,500	6,500	**10,000**	2,640	5,360	**8,000**
Maintenance	2,173	4,219	**6,392**	3,500	6,500	**10,000**	2,475	5,025	**7,500**
Scholarships	5,668	11,002	**16,670**	17,500	32,500	**50,000**	14,850	30,150	**45,000**
Consultants	0	0	**0**	0	0	**0**	0	0	**0**
Renovation	0	0	**0**	0	0	**0**	0	0	**0**
Other (Specify)			**0**			**0**			**0**
Communications	524	1,018	**1,542**	1,750	3,250	**5,000**	1,650	3,350	**5,000**
Printing	152	295	**447**	350	650	**1,000**	330	670	**1,000**
			0			**0**			**0**
Total Non-Personnel	**15,116**	**29,342**	**44,458**	**53,500**	**93,521**	**147,021**	**50,190**	**90,076**	**140,266**
GRAND TOTAL	**303,365**	**588,884**	**892,249**	**537,200**	**991,821**	**1,529,021**	**405,600**	**811,666**	**1,217,266**
Revenue									
New State Appropriation		792,061	**792,061**		773,015	**773,015**		811,666	**811,666**
Carryover State Appropriation		15,629	**15,629**		218,806	**218,806**			**0**
New Matching Funds	405,600		**405,600**	405,600		**405,600**	405,600		**405,600**
Carryover from Previous Matching	29,365		**29,365**	131,600		**131,600**			**0**
Total Revenue	**434,965**	**807,690**	**1,242,655**	**537,200**	**991,821**	**1,529,021**	**405,600**	**811,666**	**1,217,266**
Net	**131,600**	**218,806**							