

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 2009-2010**

September 28, 2010

Director:

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Executive Summary

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its fifth year of operation. These initial years have been the cornerstone in terms of the establishment and development of an effective operation. This period has continued as a time for inculcating a culture of the securing external funding as an outcome of seed research funding provided by CEACSE. There have been and continue to be some challenges as the Center is fully operational. One continuing issue is the necessity to promote and stimulate grant competition from a broader spectrum of individuals and technological areas. This is partially affected by current teaching demands or partially by other research demands. For the most part though the reporting year has proceeded smoothly with the majority of 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 received external funding from various agencies, companies, and governmental entities. The total of the awards was more than a seven and one half to one return on the monies provided to CEASE this past fiscal year (Figure 1).

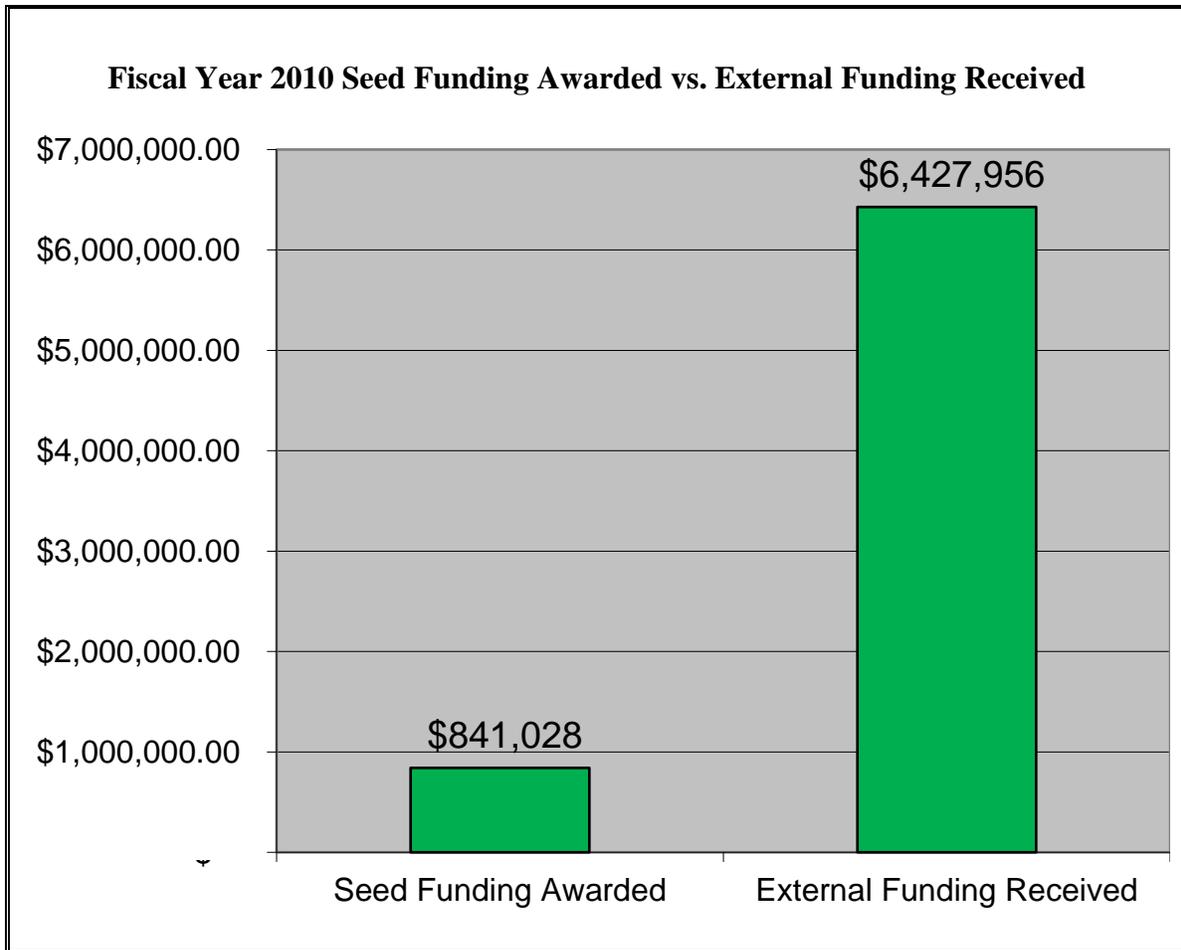


Figure 1

CEACSE continues to enhance the education 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. Both graduate and undergraduate students 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, the local companies continue to have interest in the student's educational programs impacted by the CEACSE research. The SimCenter: National Center for Computational Engineering 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 area.

The following is the Annual Report for Fiscal Year 2010 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 this 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 enlargement continues to seek 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 selected are of interest to local and national industries and state and federal agencies. While funding for the Center seeds these activities, it anticipates that significant augmentation of the state funding would result from federal grants and contracts in view of the expected wide interest in the resulting capability to solve problems of national interest. As a note, there is increased awareness by the undergraduate students of the activity of researchers and the potential of interaction.

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 technology 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 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 broadens 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 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: National Center for Computational Engineering with its expertise in computational science 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 for experienced computational engineers with appropriate guidance to learn and adapt to simulations in new physical disciplines than it is for discipline experts without computational experience to learn and adapt to computational simulation. Consequently, 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, can be very effective in generating new 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 Technology 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. In past years the cluster has achieved a significant rating when compared to other such supercomputers nationally and worldwide. However, based on the June 2010 TOP500 Supercomputer Site Rankings, UTC is no longer ranked in the Top 500. The ranking of the SimCenter cluster significantly decreased from the previous years as other organizations and universities around the world have upgraded their equipment, and should not be seen as a decrease in computing capability. With additional funding, the SimCenter could stay competitive and once again rank among the Top 500.

Of importance, is the utilization of the machines capacity. The computational speed of a machine alone does not assure significance of research results or research undertaken. The intellectual capacity of the research, blended with computational configurations of the machine is the key elements to results.

In order to meet this primary objective, 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. During this most recent year of operation it can be seen that the Center's funded activities and philosophy are continuing to achieve results (Table 1).

At the start of its fifth year, CEACSE granted funding to fifteen proposed research projects. In addition, several exploratory research activities were approved and funded during Fiscal Year 2010 (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 of several of these opportunities being identified throughout the course of the fiscal year, and thus outside the standard award cycle, these research activities were initiated at the discretion of the Center's Director. During this past fiscal year the Center has also provided funding for numerous graduate and undergraduate student research efforts.

Table 1
CEACSE Seed Funding Committed for FY 2009-2010 Research Activities

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Numerical Simulation of Lithium-Ion Batteries	\$75,833	Y	\$34,299	N	N	
Large Eddy Simulation of Internal Turbulent Flows	\$78,464	Y	\$55,179	Y	Pending	Air Force, \$1.35 million*
Implementation of the Hydrodynamic and Control System Design Technology into the Tenasi Unstructured Flow Solver	\$38,897	Y	\$22,594	N	N	
Development and Analysis of Solution Algorithms for Field Simulation Problems	\$102,075	N	98,044	Y	Y	Air Force, \$1.35 million* , pending B & W Technical Services Y-12, \$191,472†
Generic Interface Methodology for Multi-Physics Applications	\$56,093	N	42,991	Y	Y	B & W Technical Services Y-12, \$191,472†
Tetrahedral Mesh Creation/Optimization Using Edge/Face Flips	\$43,359	N	\$43,110	Y	Y	Technology used in all proposals using grid generation
Unstructured Elliptic Smoothing	\$43,359	N	\$43,316	Y	Y	Technology used in all proposals using grid generation
CFD Based Two-Phase Loss Analysis for Solid Rocket Motors	\$36,193	N	\$36,193	Y	Y	B & W Technical Services Y-12, \$191,472†
Robust and Efficient Rate Adaptation in Vehicle Ad-hoc Networks	\$50,000	N	48,000	Y	Pending	NSF
Validation of Rotorcraft Simulations using Tenasi	\$37,217	N	\$18,415	N	N	
Simulations of Interactions Between Multiple Moving Bodies Using Overset Techniques	\$52,721	N	\$31,522	Y	Y	ONR, \$480,000
Petro-Galerkin and Discontinuous Galerkin Methods for Unstructured Flow Solvers	\$83,519	N	\$49,493	Y	Y	ARMY SMDC, 1.26 million*
Diffuse Interface Methods for Wind-Ocean Wave Interactions	\$53,298	N	\$45,799	N	N	
Tank Sloshing Simulations in Microgravity Environments	\$40,000	N	\$39,706	N	N	
Emerging Infectious Disease: A Computational Multi-agent Model	\$50,000	N	\$46,580	Y	Y	NSF, \$23,000; Oak Ridge Lab, \$17,746; NSF, \$99,985; NSF, \$170,000 pending

*Single Proposal submitted to the Air Force in the amount of \$1.35 million

†Single Proposal awarded from B&W Technical Services Y-12 in the amount of \$191,472

Table 2
CEACSE Exploratory Research Activities for FY 2009-2010

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Computational Geometry Pre-processing		N	\$30,285	N	N	
Mesh Refinement/De-Refinement Strategies		N	\$16,317	N	N	
Alternate Unstructured Grid Generation Strategies		N	\$16,436	N	N	
Coupling of Global/Local Atmospheric Models		N	\$10,250	N	N	
Enhanced Agent Based Modeling		N	\$9,500	N	N	
Atmospheric Chemistry Modeling		N	\$12,335	N	N	
Discrete Event Modeling		N	\$9,375	N	N	
Relative Motion Meshes for Hydrodynamic simulations		N	\$30,488	N	N	
Higher-Order Spatial Discretization Schemes		N	\$8,750	N	N	
Validation of Free Surface Hydrodynamics		N	\$50,828	N	N	
LNG Atmospheric Dispersion		N	\$31,825	N	N	
Turbomachinery Applications		N	\$5,103	N	N	
Novel Algorithm Development		N	\$19,728	N	N	
Aerodynamic Drag Reduction Devices		N	\$31,874	N	N	

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, mid-term 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 has 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 19 faculty members from various disciplines, such as physics, computer science, and computational engineering,

CEACSE funding has continued the support of seven Ph.D. graduate students, five Masters level graduate students, and eight undergraduate students. One Masters level student who worked on a grant graduated in May 2010 and is currently pursuing

his Ph.D. at The University of Tennessee at Chattanooga. A current Ph.D. student is teaching at the University of Tennessee at Chattanooga. Masters level students, working together on a seed funded research projects, continue to present their research work at major conferences.

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 five years, CEACSE faculty have made at least 150 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. 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. A journal article was published based on research on improving fuel economy of large trucks by reducing aerodynamic drag, in support of two Chattanooga companies. According to U.S. Xpress President Max Fuller, this work

allowed his company, one of the nation's largest trucking firms, to save 10% or \$68.4M per year in fuel bills. Technical input on drag reduction for slotted mud flap designs is also expected to produce improved Eco-flap designs and increased sales for Anderson Flaps, Inc. The article appeared in *Computers and Fluids* in September 2009:

D. G. Hyams, K. Sreenivas, R. Pankajakshan, D. S. Nichols, W. R. Briley, D. L. Whitfield. "Computational Simulation of Model and Full-Scale Class 8 Trucks with Drag Reduction Devices", *Computers and Fluids*, 2009

2. The SimCenter has joined in a partnership with Tuftco Corporation in Chattanooga. This small manufacturing company designs and manufactures machines that make carpet, taking yarn from tufting to finished carpet. The SimCenter and Tuftco's engineering design staff have an established working relationship based on the SimCenter's past use of M&S to help Tuftco resolve a major energy-cost design problem with a machine based on a new technology that was otherwise highly successful. After two separate attempts with low-fidelity models did not uncover the source of the severe energy losses, high-fidelity simulations of the airflow system were used successfully to generate design modifications that reduced the overall energy consumption to 1/3 of the original design (400 hp to 135 hp). Tuftco Corporation has agreed to participate in one of the planned Pilot Projects, which would use high-fidelity simulations early in the design process for Tuftco's next-generation carpet manufacturing machine.

3. The SimCenter has joined in a partnership with TrailManor, located in Lake City, TN. TrailManor manufactures uniquely-designed lightweight recreational travel trailers that are easily towed by moderately sized 6-cylinder family vehicles. The SimCenter has performed some airflow simulations for complex geometries consisting of one of their trailers, a minivan, and the combination of the trailer being towed by the minivan. This feasibility study has established the potential for using high-fidelity simulations to develop improved trailer designs. TrailManor is enthusiastic about participating in one of the planned Pilot Projects, which would use high-fidelity airflow simulations to develop an improved trailer design with modifications that will reduce aerodynamic drag and thereby increase gas mileage, with potentially significant energy savings.

4. Officials and representatives in Chattanooga, recently inaugurated the City's first Bloom Box, a 100kW energy server poised to become an important alternative energy source for the nation's power grid. The project is the continuation of a long-standing partnership between the SimCenter, EPB, TVA, and Bloom Energy that began with Bloom's first field trial of its technology in 2006. Located on the top floor of the EPB building's parking garage, in downtown Chattanooga, the Bloom Box will be a showcase piece for innovation and for successful collaboration between the public and private sectors. By working closely with TVA, this project also highlights how distributed generation technologies such as Bloom's can be an integral part of

a clean smart grid for the 21st century. The units will be closely monitored by EPB, Bloom Energy, and the SimCenter to optimize and simulate performance and to provide educational value of cutting edge energy technology.

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.

The Center has worked to define the nature of educational outreach activities that would work to create awareness and stimulate interest in science and engineering among pre-college students. During this past year, the SimCenter conducted several events for local schools, partnering with other departments on campus and even had a high school junior intern at the Center this summer preparing grids and running flow solutions on geometries of interest. The center hosted over 200 students from Soddy-Daisy Middle, Red Bank High School, Signal Mountain High School, Central High School, Battle & Brown Elementary Schools, and Southern Adventist University. Also, the SimCenter hosted a week-long inter-session activity with Chattanooga Girls Leadership Academy and summer camps with the Urban League, International Youth Services Foundation, and Girls, Inc. Students were shown how the SimCenter actually uses mathematical models to simulate real-world problems and then compare the results with real experiments. Several group activities were conducted, with culminating events such as a paper airplane design fly-offs, a fuel cell powered car race, and a trip to the Raccoon Mountain pumped storage facility. The purpose is to stimulate early student interest in math and science courses that will prepare them for possible STEM majors upon entering college.

Additionally, the SimCenter provided presentations to almost fifty high-achieving high school juniors and seniors participating in the Governor's School for Computational Physics which was held at Austin Peay State University. The tour of the SimCenter and the faculty presentations were one of three such events that the students were able to experience, also touring computational facilities at NASA Marshall in Huntsville, Alabama and at Oak Ridge National Laboratory. By invitation of the Creative Discovery Museum of Chattanooga, the SimCenter has collaborated with the children's museum on several occasions to produce exhibits that would appeal to young children interested in Math and Science. Additional types of outreach will continue to be investigated since these activities with elementary, middle and high schools continue to be softer than desired. With partnerships that are being forged with many local schools and organizations (i.e., we have a seat on the STEM advisory board of the Urban League and have been working on the science curriculum with CSAS), more contact time and thus more depth of content are on the horizon.

UTC undergraduates have been recruited to work and are part of ongoing funded research projects, and this effort is continuing. Eight undergraduates have been employed as research assistants through the most recent fiscal year. Planning efforts continue to identify and develop additional effective outreach activities for undergraduate and graduate students, although the inclusion of an engineering course in the UHON department (UHON 1200, Spring 2011) and a teaching presence in the undergraduate design classes has already gone a long way in spurring interest. Finally, the MODSIM 2010 conference in Virginia, co-chaired by a SimCenter staff

member, will be an invaluable resource in not only making more STEM connections but also in learning others' techniques and collaborating on activities (such as the NASA RWIW program).

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.

1. Numerical Simulation of Lithium-Ion Batteries

- Principal Investigator(s): Dr. Kyle Anderson and Dr. Sagar Kapadia, Graduate School of Computational Engineering
- Objective(s): To develop computational methods for simulating lithium-ion batteries and to develop an initial simulation capability for analysis. This will then be extended to modeling combustion. Sensitivity derivatives will also be obtained for examining effects of physical parameters.
- Seed Funding: \$75,833
- Results: Continuing-Technology is still under development.

2. Large Eddy Simulation of Internal Turbulent Flows

- Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
- Objective(s): To develop, implement, and evaluate the accuracy of models to perform large-eddy simulation of internal turbulent flows in realistic engineering configurations.
- Seed Funding: \$78,464
- Results: Technology developed and demonstrated. This resulted in a proposal to the Air Force in the amount of \$1.35 million. Award notification is pending at time of report.

3. Implementation of the Hydrodynamic and Control System Design Technology into the Tenasi Unstructured Flow Solver

- Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
- Objective(s): To implement and evaluate the hydrodynamic/aerodynamic and control system design technology into the Tenasi unstructured flow solver.
- Seed Funding: \$38,897
- Results: Continuing—Technology is still under development.

4. Development and Analysis of Solution Algorithms for Field Simulation Problems

- Principal Investigator(s): Dr. Roger Briley and Dr. David Whitfield, Graduate School of Computational Engineering
- Objective(s): To conduct exploratory research on improved methods for solving field conservation/balance equations that may include complex and/or stiff source terms.
- Seed Funding: \$102,075

- Results: Technology developed was used in pending \$1.35 million proposal to the Air Force and also a \$191,472 proposal to B & W Technical Services Y-12.

5. Generic Interface Methodology for Multi-Physics Applications

- Principal Investigator(s): Dr. Daniel Hyams, Graduate School of Computational Engineering
- Objective(s): To establish a computational foundation to allow for the communication of generic entities across volume boundaries, which would allow for simulation of the interaction and response of an overall system.
- Seed Funding: \$56,093
- Results: Technology developed and undergoing testing. This resulted in a \$191,472 proposal to B & W Technical Services Y-12. A future proposal is awaiting a BAA in Heat Transfer.

6. Tetrahedral Mesh Creation/Optimization Using Edge/Face Flips

- Principal Investigator(s): Dr. Steve Karman, Graduate School of Computational Engineering
- Objective(s): Implementation of a tetrahedral mesh creation procedure using point insertion combined with edge and face flips to optimize the mesh quality based on cost function.
- Seed Funding: \$43,359
- Results: Technology developed and utilized in all proposals that have required grid generation.

7. Unstructured Elliptic Smoothing

- Principal Investigator(s): Dr. Steve Karman, Graduate School of Computational Engineering
- Objective(s): Extend the initial stencil of the VCV method to incorporate control of edge lengths as well as angles of the faces of control volume.
- Seed Funding: \$ 43,359
- Results: Technology developed and utilized in all proposals that have required grid generation.

8. CFD Based Two-Phase Loss Analysis for Solid Rocket Motors

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To use the Lagrangian particle module in UTC Tenasi with enhancements to study the sources and magnitudes of two-phase losses in solid rocket motors.
- Seed Funding: \$36,193

- Results: The Lagrangian particle module resulted in a \$191,472 proposal to B & W Technical Services Y-12. A future proposal is awaiting a BAA for Solid Rocket Motors.

9. Robust and Efficient Rate Adaptation in Vehicle Ad-hoc Networks

- Principal Investigator(s): Dr. Mina Sartipi, Computer Science and Engineering
- Objective(s): To maintain the optimal performance of wireless communications in vehicle networks. Three modern channel codes will be tested and evaluated for this application: wavelet convolutional codes, LDPC codes, and rateless codes.
- Seed Funding: \$50,000
- Results: Proposal submitted to NSF and another proposal is being prepared for submission to DARPA.

10. Validation of Rotorcraft Simulations using Tenasi

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): To validate the unstructured variant of Tenasi in simulating rotorcraft problems.
- Seed Funding: \$37,217
- Results: Technology developed and undergoing testing. A future proposal is awaiting a BAA in this topic area.

11. Simulations of Interactions Between Multiple Moving Bodies Using Overset Techniques

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): To implement a method that will be capable of handling interactions between multiple moving bodies without necessitating grid regeneration.
- Seed Funding: \$52,721
- Results: Technology developed and demonstrated. The technology was utilized in a \$480,000 grant from ONR .

12. Petro-Galerkin and Discontinuous Galerkin Methods for Unstructured Flow Solvers

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): To explore the Petrov-Galerkin and Discontinuous Galerkin methods for improving the accuracy of the unstructured flow solver.
- Seed Funding: \$83,519

- Results Technology developed and demonstrated. The technology is utilized in the \$1.26 million contract from ARMY SMDC.

13. Diffuse Interface Methods for Wind-Ocean Wave Interactions

- Principal Investigator(s): Dr. Lafayette Taylor, Graduate School of Computational Engineering
- Objective(s): To develop a Diffuse Interface of Method that fully accounts for the mutual interaction between atmospheric winds and ocean waves.
- Seed Funding: \$53,298
- Results: Theoretical development completed. Implementation and testing on specific applications necessary before proposal preparation.

14. Tank Sloshing Simulations in Microgravity Environments

- Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): To perform code development, physical modeling and simulations for tank sloshing in a microgravity environment, using the Tenasi flow solver.
- Seed Funding: \$40,000
Results: Technology developed and demonstrated. A future proposal is awaiting a BAA in this topic area.

15. Emerging Infectious Disease: A Computational Multi-agent Model

- Principal Investigator(s): Dr. Li Yang, Computer Science and Engineering
- Objective(s): To examine the effect of various factors and interaction situation on emergent epidemic patterns on infectious diseases.
- Seed Funding: \$50,000
Results: \$23,000 grant funded by NSF; \$17,746 grant awarded by Oak Ridge National Laboratory; \$99,985 grant awarded by NSF; \$170,000 pending grant by NSF.

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.

**Allocation of CEACSE Funding
Fiscal Year 2010**

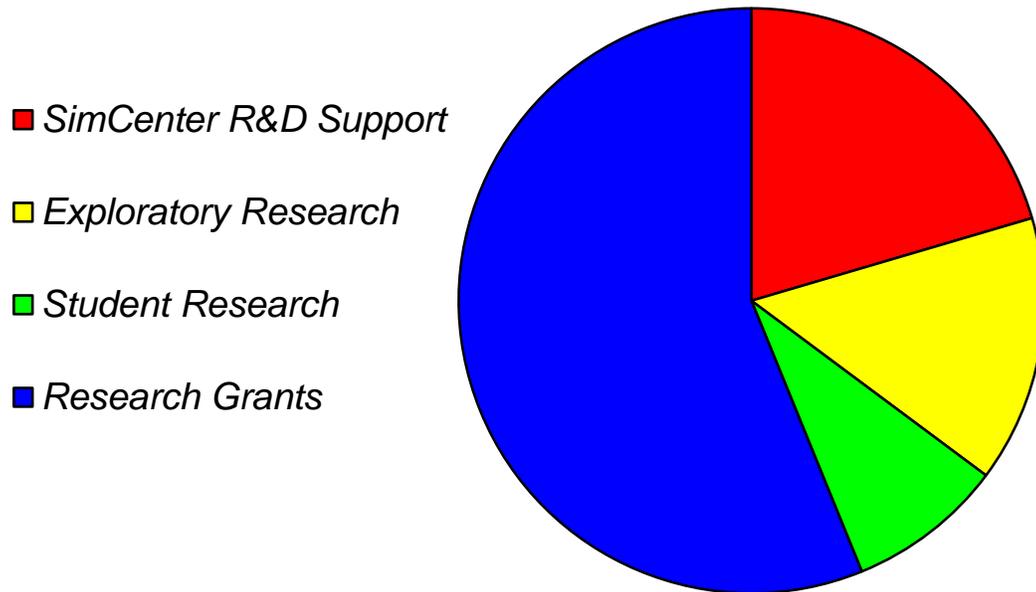


Figure 2

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:	\$ 4,765,984
External Funding Awarded in Fiscal Year 2009-2010:	\$ 6,427,956
Total External Funding Awarded:	\$18,535,847

* 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 three-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 FY10. This performance has been consistent and CEACSE works toward continuous improvement.

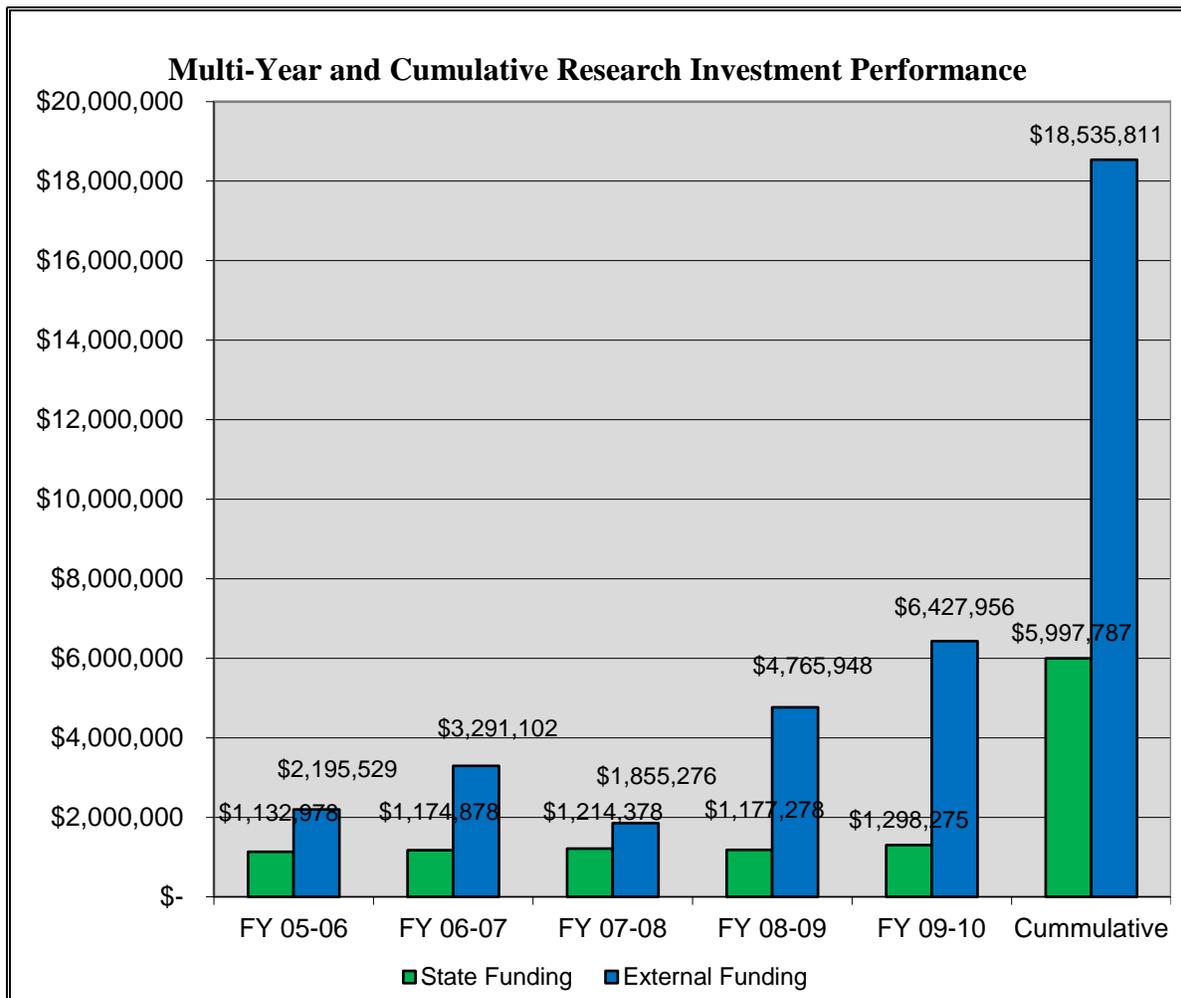


Figure 3

FY 2010 Publications and Presentations of the Center's Research Activities

1. Ji, L., Sreenivas, K., Hyams, D., and Wilson, R., "A Parallel Universal Mesh Deformation Scheme for Hydrodynamic Applications," Proceedings of the 28th ONR Symposium on Naval Hydrodynamics, Pasadena, CA, 12-17 Sep. 2010.
2. Hyams, D. G., Webster, R. W., and Sreenivas, K., "A Generalized Interpolative Interface for Parallel Unstructured Flow Solvers," 40th Fluid Dynamics Conference and Exhibit, Chicago, Illinois, June 28-1, 2010. Paper No. 2010-5097.
3. Hyams, D. G., Webster, R. W., and Sreenivas, K., "A Generalized Axisymmetric Boundary Condition Method for Parallel Unstructured Field Solvers," Proceedings of ASME Gas Turbine Technical Congress and Exposition 2010, Glasgow, UK, June 14-18, 2010. Paper GT2010-23414.
4. Ji, L., Wilson, R., Sreenivas, K., and Hyams, D., "A Parallel Universal Mesh Deformation Scheme," 28th AIAA Applied Aerodynamics Conference, June 2010, Chicago, AIAA-2010-367.
5. Kapadia S., Anderson W.K., Workman N., "Computational Design of Tubular Solid Oxide Fuel Cells," ASME 2010 8th International Fuel Cell Science, Engineering & Technology Conference, June 14-16, 2010, Brooklyn, New York.
6. Li Wang, Dimitri J. Mavriplis and W. Kyle Anderson, "Unsteady Discrete Adjoint Formulation for High-order Discontinuous Galerkin Discretizations in Time-dependent Flow Problems", 48th AIAA Aerospace Science Meeting, January 2010, Orlando, FL, AIAA-2010-367.
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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 secured from the activities of the Center. This should continue into the future.

There have been increased activities in both direct and indirect support of economic development for Tennessee. There have been a number of meeting 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 needs 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 succeeding in leveraging 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 is 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 UT Chattanooga Center Center of Excellence in Applied Computational Science & Engineering

	FY 2008-09 Actual			FY 2009-10 Proposed			FY 2010-11 Requested		
	Matching	Appopr.	Total	Matching	Appopr.	Total	Matching	Appopr.	Total
Expenditures	357,578	819,700	1,177,278	357,578	811,200	1,168,778	357,578	851,760	1,209,338
Salaries									
Faculty	187,477	437,447	624,924	227,010	477,990	705,000	189,440	450,560	640,000
Other Professional	18,955	44,228	63,183	22,218	46,782	69,000	18,352	43,648	62,000
Clerical/ Supporting	2,179	5,085	7,264	4,830	10,170	15,000	2,960	7,040	10,000
Assistantships	47,701	111,302	159,003	67,620	142,380	210,000	51,800	123,200	175,000
Total Salaries	256,312	598,061	854,373	321,678	677,322	999,000	262,552	624,448	887,000
Longevity	104	244	348	161	339	500	178	422	600
Fringe Benefits	53,910	125,790	179,700	92,493	194,753	287,246	77,978	185,462	263,440
Total Personnel	310,326	724,095	1,034,421	414,332	872,414	1,286,746	340,708	810,332	1,151,040
Non-Personnel									
Travel	6,143	14,334	20,478	7,084	14,916	22,000	5,920	14,080	20,000
Software	1,500	3,500	5,000	483	1,017	1,500	444	1,056	1,500
Books & Journals	19	45	64	24	51	75	22	53	75
Other Supplies	15	35	51	354	746	1,100	355	845	1,200
Equipment			0			0			0
Maintenance			0			0			0
Scholarships	10,330	24,104	34,435	17,710	37,290	55,000	8,880	21,120	30,000
Consultants	4,500	10,500	15,000	4,780	10,220	15,000	1,250	2,973	4,223
Renovation			0			0			0
Other (Specify)			0			0			0
Communications	378	882	1,260	419	881	1,300	385	915	1,300
			0			0			0
Total Non-Personnel	22,886	53,401	76,287	30,854	65,121	95,975	17,256	41,042	58,298
GRAND TOTAL	333,212	777,495	1,110,708	445,186	937,535	1,382,721	357,964	851,374	1,209,338
Revenue									
New State Appropriation		819,700	819,700		811,200	811,200		851,760	851,760
Carryover State Appropriation		84,130	84,130		126,335	126,335			0
New Matching Funds	357,578		357,578	357,578		357,578	357,578		357,578
Carryover from Previous Matching	63,242		63,242	87,608		87,608			0
Total Revenue	420,820	903,830	1,324,650	445,186	937,535	1,382,721	357,578	851,760	1,209,338