

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

**CENTER OF EXCELLENCE**

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**IN APPLIED COMPUTATIONAL  
SCIENCE AND ENGINEERING**

**Annual Report to the  
Tennessee Higher Education Commission  
Fiscal Year 2007-2008**

*September 22, 2008*

Director:

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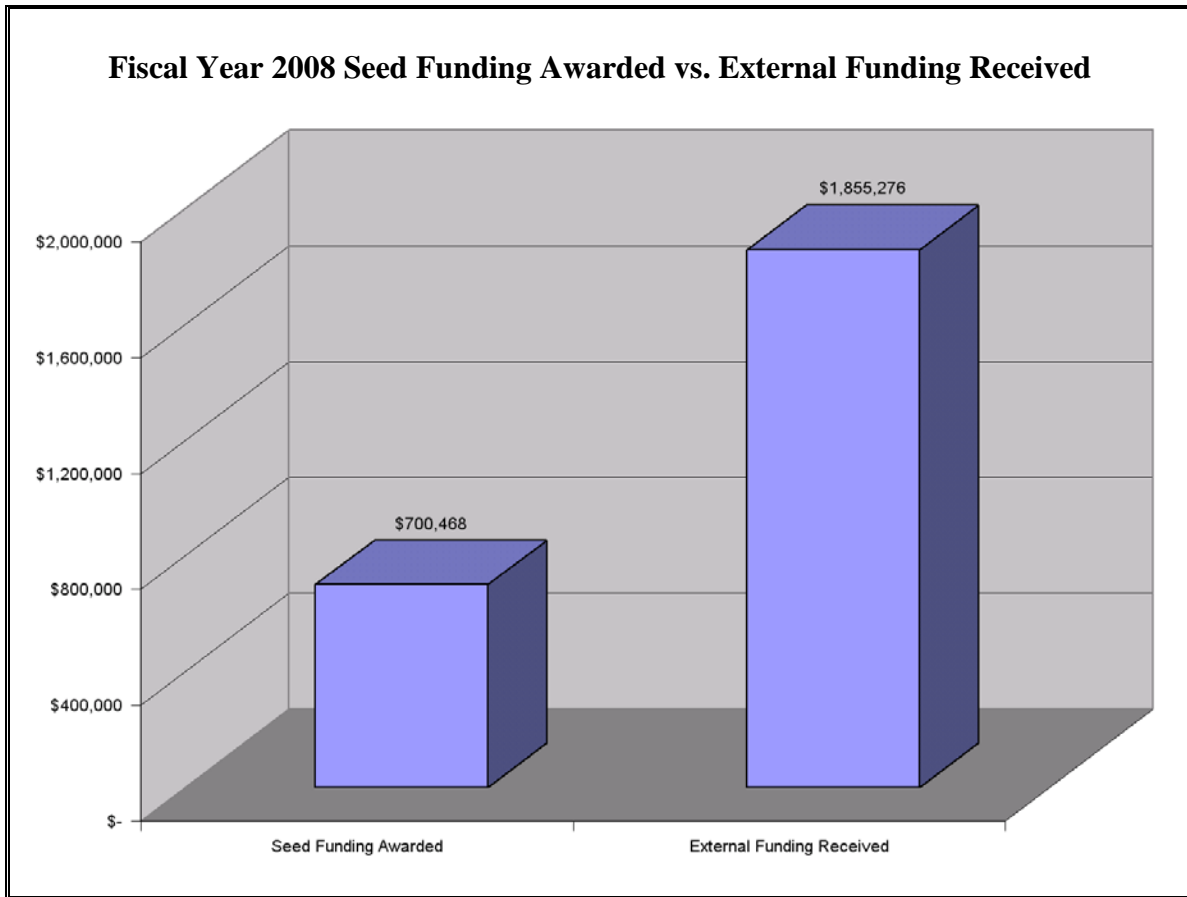
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## **Executive Summary**

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its third year of operation. These initial years have been the cornerstone in terms of the establishment and development of an effective operation. This also has been a period of 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 challenge is the necessity to provide extensions to researchers who were awarded seed funding during the previous fiscal years. This reporting year has proceeded smoothly with the majority of the awarded research funds being expended. Seven funded research projects were granted extensions to allow them to complete their research.

As is noted in this report, CEACSE continues to accomplish its mission and objectives. Through the awards, the researchers and their academic units have received funding from various agencies, companies, and governmental entities. The total of the awards exceeded a two-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 been utilized on various research activities undertaken as a result of CEACSE funding. Due to the research activities that some of the students have undertaken, the students are progressing through their educational programs with the aid of funding by local companies impacted by the CEACSE research. The SimCenter: National Center for Computational Engineering continues to be an anchor and attract students locally as well as nationally and internationally.

As stated in previous reports, as a result of funding research activities and secured external funding, several companies are now operating offices here in the Chattanooga area. At least one company has progressed to initiating new manufacturing operations in Tennessee. This component of CEACSE's objectives is a continuing effort. As CEACSE's activities and accomplishments continue to develop, this component should gain additional traction in economic development.

The following is the Annual Report for Fiscal Year 2008 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 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.

### **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 2008 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.

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 third year, CEACSE granted seed funding to fifteen proposed research projects. In addition, several exploratory research activities were approved and funded during Fiscal Year 2007 (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, 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 2007-2008 Research Activities***

<b>Project Title</b>	<b>Budget</b>	<b>One-Year Extension</b>	<b>Expenses</b>	<b>Proposal Submitted</b>	<b>Externally Funded</b>	<b>External Funding Source(s)</b>
Entanglement, Decoherence, and Quantum Feedback	\$ 25,000		\$ 10,818	Y	N	
Multicast Protocol on Intel Mote 2 Sensor Network Platform	\$ 35,000		\$ 36,280	Y	Y	Wheeler Center for Odor Research
A Secure and Reliable Wireless Ad-Hoc Network in Disaster Management	\$ 20,000		\$ 20,242	Y	Y	DoD-IASP Scholarship program Odor Wheeler Foundation
Simulation of Biodiesel Production by Microreaction Systems	\$ 25,000	Y	\$ 17,796	N	N	
Analysis and Sensitivity Derivatives for Plasma Simulations	\$ 57,500	Y	\$ 43,010	N	N	
Computational Analysis and Design of Fuel Cell Components	\$ 25,000		\$ 24,944	Y	Y	Office of Naval Research
Adjoint-Based System for Design Optimization	\$ 160,000	Y	\$ 76,399	N	Y	NASA Glenn Research Center, 2 <sup>nd</sup> Year funding
Physical/Mathematical Modeling and Solution of Field Simulation Problems	\$ 100,000	Y	\$ 81,805	N	N	
A Droplet Splatter Model for the Tenasi Particle Module	\$ 34,000		\$ 26,497	Y	Y†	ERC, Inc./Air Force Research Lab†
An Agent-Based Simulation Module in Tenasi	\$ 34,000		\$ 26,393	Pending	N	
Turbulence Modeling for Multi-Speed Flows	\$76,500	Y	\$ 59,592	N	N	
Development of a Deforming Mesh Capability for Unstructured Meshes	\$53,500		\$ 39,464	Y	Y	Aerotomy, Inc.
Kinetic Simulation of Chemically Reactive Gas Flows on Unstructured Grids	\$89,000		\$ 89,634	N	N	
Hybrid Turbulence Models for Vortex and Separated Flows	\$86,500	Y	\$ 69,906	Pending	N	
Modeling and Analysis of Combustion Instability in Rocket Engines and Motors	\$106,600	Y	\$ 77,689	Y	Y†	ERC, Inc./Air Force Research Lab†

† Official Award Notification is pending

**Table 2**  
**CEACSE Exploratory Research Activities for FY 2007-2008**

<b>Exploratory Research Activities</b>	<b>Budget</b>	<b>One-Year Extension</b>	<b>Expenses</b>	<b>Proposal Submitted</b>	<b>Externally Funded</b>	<b>External Funding Source(s)</b>
Discretization and Basic Algorithms for the Equations Governing Electromagnetics and Plasmas		Y	\$ 1,324.59	N	N	
Large Eddy Simulations of Chemically Reacting Flows		Y	\$ 12,352.49	N	N	
Full Reynolds stress simulations for compressible flows		Y	\$ 8,235.00	N	N	
Chemically reacting flow simulations for combustion and high speed regimes		Y	\$ 60,213.70	N	N	
Chemically reacting flow simulations for diffusion flames		Y	\$ 1,232.70	N	N	
Generalized grid motion and deformation algorithms		Y		N	N	
Multiphase flow formulations for chemically reacting flows		Y		N	N	
Turbomachinery simulations with advanced turbulence models		Y	\$ 4,249.31	N	N	
Chemically reacting flow simulations for combustion		Y	\$ 2,832.88	N	N	
Simulation and analysis of acoustics associated with combustion		Y	\$ 2,360.73	N	N	
Formulation of advanced turbulence models including Wall Modeled Large Eddy Simulation		Y	\$ 5,264.49	N	N	
Formulation of Phase-Field methods for diffuse fluid interface modeling		Y	\$ 9,476.08	N	N	
Formulation of models for highly vortical flows		Y	\$ 6,317.38	N	N	
Simulations of fluid structure interaction for ships in varying sea states		Y	\$ 5,244.25	N	N	
Formulation of alternate free surface flow models		Y	\$ 3,496.17	N	N	
Simulations to Reduce Aerodynamic Drag of Heavy Vehicles		Y	\$ 821.80	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 21 faculty members from various disciplines, such as physics, computer science, and computational engineering, including one Masters level student and one Ph.D. level student who are also staff members.

CEACSE funding has continued the support of eight Ph.D. graduate students, twelve Masters level graduate students, and nine undergraduate students. One Ph.D. student working under a seed grant graduated in August 2008 and has accepted a research faculty position at the University. A second Ph.D. student graduated in August 2008 and has accepted a research position with a local corporation. One Masters level student who worked on a seed grant graduated in August 2008 and is currently pursuing his Ph.D. at The University of Tennessee at Chattanooga. Two Masters level students, working together on a seed funded research project, presented their research work at the 2008 ACM Middle-Southeast Annual Conference. One of those students was awarded first place for the Masters student paper awards out of a number of universities in Tennessee, Alabama, Georgia and Mississippi.

*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 three years, CEACSE faculty have made at least 75 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, during the past year, CEACSE sponsored research (Projects 6, 7, 8, 11, 12, and 14) has directly or indirectly enabled the following activities at the SimCenter that are supportive of economic development:

1. The SimCenter has provided and is currently providing a considerable amount of technical input to U.S. Xpress Enterprises, Inc., one of the nation's largest trucking firms and a Chattanooga based company, to help them to make informed choices for the short-list of devices to be internally road tested and introduced into the fleet. These results promise very substantial improvement in fleet fuel economy. U.S. Xpress President Max Fuller said his company will save 10% or \$68.4M per year in fuel bills. Related SimCenter work for Anderson Flaps, Inc. of Chattanooga to help assess their Eco-flap designs (slotted mud flaps) for drag reduction indicate improvement for sufficient magnitude to justify modifications, and this should lead to increased Eco-flap sales.
2. The SimCenter has a close partnership with a Huntsville-based emerging technology firm Radiance Technology, Inc., who opened a new project office in Chattanooga with eight engineers. Radiance and the SimCenter have a government-sponsored research collaboration in electromagnetics. Radiance has hired two SimCenter Ph.D. students who graduated this year. This is a significant event because the SimCenter partnership with Radiance has produced new jobs that allow two of our graduates to remain in Chattanooga.

3. The SimCenter has a partnership with Aerotonomy, Inc., a small business in Atlanta, GA to provide modeling and simulation support for their design of a synthetic-jet controlled wing design for UAV aircraft, under Air Force SBIR sponsorship. This is a new application area for the SimCenter that will offer future funding opportunities.
4. The SimCenter has a partnership with the Chattanooga Enterprise Center in connection with the SimCenter's joint research on Solid Oxide fuel cells with Bloom Energy of California. There is a potential Chattanooga can secure a share of the ultimate manufacturing business for this fuel cell, based on this relationship.
5. The Chattanooga Chamber of Commerce asked the SimCenter to help assess whether prevailing winds across Hamilton County would transport dust from detonations at the Vulcan and AMT quarries in Chattanooga to the new Enterprise South site. SimCenter simulations indicated that this was unlikely to be a problem, and there is a reasonable probability that this issue arose during recent negotiations with Volkswagen. There is a potential for a future SimCenter relationship with Volkswagen in existing research areas such as truck drag reduction and possibly new areas.
6. The SimCenter assisted engineers from Mohawk Industries, Inc., a carpet manufacturer in Dalton GA, in their effort to solve a manufacturing problem with cooling of extruded carpet fibers. There is potential for future collaboration with Mohawk regarding other areas of research.



*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 the first of a planned series of all-day events for the Math Counts program in which over 20 students from Tyner Middle School were shown how the SimCenter actually uses mathematical models to simulate real-world problems and then compare the results with real experiments. 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.

UTC undergraduates have been recruited to work and are part of ongoing funded research projects, and this effort is continuing. Nine undergraduates have been employed as research assistants through the most recent fiscal year. Also, representatives from Southern Adventist University of Collegedale, TN visited the SimCenter to learn more about the Center and to discuss how to interest and prepare their students to enter our Computational Engineering graduate program. Planning efforts continue to identify and develop additional effective outreach activities for undergraduate and graduate students.

### ***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. Entanglement, Decoherence, and Quantum Feedback**

- Principal Investigator(s): Dr. Jin Wang, Physics
- Objective(s): To show how entanglement increases as the atom-cavity joint decoherence rate increases in the presence of optimal feedback, in order to show the upper limit of entanglement creation.
- Seed Funding: \$ 25,000
- Results: Dr. Wang submitted proposals for external funding to the National Science Foundation and the University of Tennessee Research Corporation. None of the proposals were funded.

**2. Multicast Protocol on Intel Mote 2 Sensor Network Platform**

- Principal Investigator(s): Dr. Mina Sartipi, Electrical Engineering
- Objective(s): To introduce a new multicasting algorithm and a simple routing protocol for lossy wireless sensor networks with a focus on reducing the power consumed by sensor nodes in transmitting data from source node to destination nodes through multiple hops.
- Seed Funding: \$ 35,000
- Results: Dr. Sartipi submitted proposals for external funding to:
  - i. The Microsoft Research New Faculty Fellowship program. This proposal was not funded.
  - ii. The William H. Wheeler Center for Odor Research, and received \$20,000.
  - iii. The National Science Foundation's Career Award program. The results of this proposal were not available at the time of the publication of this report.

**3. A Secure and Reliable Wireless Ad-Hoc Network in Disaster Management**

- Principal Investigator(s): Dr. Li Yang and Dr. Joseph Kizza, Computer Science
- Objective(s): To design an infrastructure-less communication model to significantly improve our ability to control damage of a disaster where geographical or terrestrial constraints demand totally distributed networks. To develop different strategies to defend the wireless networks against misbehaving nodes in harsh environments. To implement the secure and reliable wireless networks for the Chattanooga Area Regional Transportation Authority (CARTA) in the short term, and The City of Chattanooga in the long term.
- Seed Funding: \$ 20,000
- Results: Dr. Yang and Dr. Kizza submitted proposals for external funding to:
  - i. The National Science Foundation IT-Start program, National Science Foundation CI-TEAM (teamed with Louisiana State University), and the Department of Defense IASP infrastructure program.. None of the proposals were funded.

- ii. The Department of Defense IASP scholarship program, and was awarded \$62,279.79.
- iii. The Odor Wheeler Foundation, and was awarded \$20,000.
- iv. The National Science Foundation SFS scholarships program. The results of this proposal were not available at the time of the publication of this report.

#### **4. Simulation of Biodiesel Production by Microreaction Systems**

- Principal Investigator(s): Dr. Frank Jones, Chemical Engineering
- Objective(s): To design and simulate a micro reaction system that produces biodiesel fuel from soybean oil.
- Seed Funding: \$ 25,000
- Results: One-Year No-Cost Extension granted to allow Dr. Jones to complete this research project. Proposals are expected to be submitted upon completion of the research project.

#### **5. Analysis and Sensitivity Derivatives for Plasma Simulations**

- Principal Investigator(s): Dr. Kyle Anderson, Graduate School of Computational Engineering
- Objective(s): To develop computational methods for numerically simulating RF capacitive-coupled discharge plasmas. To develop simulation capability that will account for reactions amongst multiple species as well as metastable molecules and elements. To obtain sensitivity derivatives with the intent of using the sensitivity derivatives in conjunction with the analysis codes to influence the plasma parameters and chemical composition to achieve particular design goals.
- Seed Funding: \$ 57,500
- Results: One-Year No-Cost Extension granted to allow Dr. Anderson to complete this research project. Proposals are expected to be submitted upon completion of the research project.

#### **6. Computational Analysis and Design of Fuel Cell Components**

- Principal Investigator(s): Dr. Kyle Anderson, Graduate School of Computational Engineering
- Objective(s): To use numerical simulations to analyze and improve fuel cell components that are considered critical for advancing the technology to the point where fuel cells become a viable means of producing power for industrial applications.
- Seed Funding: \$ 25,000
- Results: Dr. Anderson submitted proposals for external funding to the Office of Naval Research and was awarded \$1,527,996.

#### **7. Adjoint-Based System for Design Optimization**

- Principal Investigator(s): Dr. Chad Burdyshaw and Dr. Kyle Anderson, Graduate School of Computational Engineering

- Objective(s): To research and develop methods to exploit the adjoint capability for error estimation and for adaptive meshing in order to significantly enhance the capability of the SimCenter to improve existing designs using computational methods.
- Seed Funding: \$ 160,000
- Results: One-Year No-Cost Extension granted to allow Dr. Burdyshaw and Dr. Anderson to complete this research project. Proposals are expected to be submitted upon completion of the research project.

#### **8. Physical/Mathematical Modeling and Solution of Field Simulation Problems**

- Principal Investigator(s): Dr. Roger Briley, Dr. David Whitfield and Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To identify new application areas in which SimCenter modeling and simulation expertise can make important contributions, to identify how existing technologies can be leveraged within these areas, and to link these opportunities to potential funding sources.
- Seed Funding: \$ 100,000
- Results: One-Year No-Cost Extension granted to allow Dr. Briley, Dr. Whitfield and Dr. Pankajakshan to complete this research project. Proposals are expected to be submitted upon completion of the research project.

#### **9. A Droplet Splatter Model for the Tenasi Particle Module**

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To design and implement a droplet splatter model to the *Tenasi* particle module for more realistic simulation of solid rocket motors, and to verify and validate the model upon implementation.
- Seed Funding: \$ 34,000
- Results: Dr. Pankajakshan contributed to a proposal for external funding to ERC, Inc and the US Air Force Research Laboratory, and is awaiting award notification of \$150,000.

#### **10. An Agent-Based Simulation Module in Tenasi**

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): Design and implementation of an agent-based model (ABM) within the *Tenasi* solver suite to be used for flooding and/or plume transport simulations, which will be used to drive evacuation simulations using the ABM module. To verify and validate the model upon implementation.
- Seed Funding: \$ 34,000
- Results: No proposals were submitted at the time of this report. Dr. Pankajakshan has completed his research in this area and is exploring possible external funding sources. Proposals are expected to be submitted in the future.

### **11. Turbulence Modeling for Multi-Speed Flows**

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering
- Objective(s): To identify and correct the root causes of intermittent inaccurate turbulent performance in the *Tenasi* code to guarantee the utmost accuracy and confidence in the turbulent Arbitrary Mach Number simulations ranging from combustion modeling to atmospheric flows.
- Seed Funding: \$76,500
- Results: One-Year No-Cost Extension granted to allow Dr. Briley, Dr. Whitfield and Dr. Pankajakshan to complete this research project. Proposals are expected to be submitted upon completion of the research project.

### **12. Development of a Deforming Mesh Capability for Unstructured Meshes**

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): To develop an algorithm capable of deforming unstructured meshes, and implement it in the unstructured variant of the Tenasi family of flow solvers in order to carry out physics based trajectory simulations that arise from prescribed movement of control surfaces on submarines, surface ships and aircraft.
- Seed Funding: \$53,500
- Results: Dr. Sreenivas submitted a proposal for external funding to Aerotonomy, Inc. and was awarded \$75,000.

### **13. Kinetic Simulation of Chemically Reactive Gas Flows on Unstructured Grids**

- Principal Investigator(s): Mr. Glenn Brook, Graduate School of Computational Engineering
- Objective(s): To extend a parallel, implicit, unstructured, finite-volume flow solver for the Boltzmann-BGK equation to support chemically reactive species.
- Seed Funding: \$89,000
- Results: No proposals were submitted at the time of this report. Mr. Brook has shifted the focus of his research slightly and proposals are expected to be submitted in the future.

### **14. Hybrid Turbulence Models for Vortex and Separated Flows**

- Principal Investigator(s): Dr. Lafe Taylor, Graduate School of Computational Engineering
- Objective(s): To implement a new hybrid turbulence model into the unstructured Tenasi CFD code for application to massively separated and vortex dominated flows. To verify and validate the numerical accuracy of this turbulence model. To establish the computational resources required for various applications.
- Seed Funding: \$86,500

- Results: One-Year No-Cost Extension granted to allow Dr. Taylor to complete this research project. Proposals are expected to be submitted upon completion of the research project.

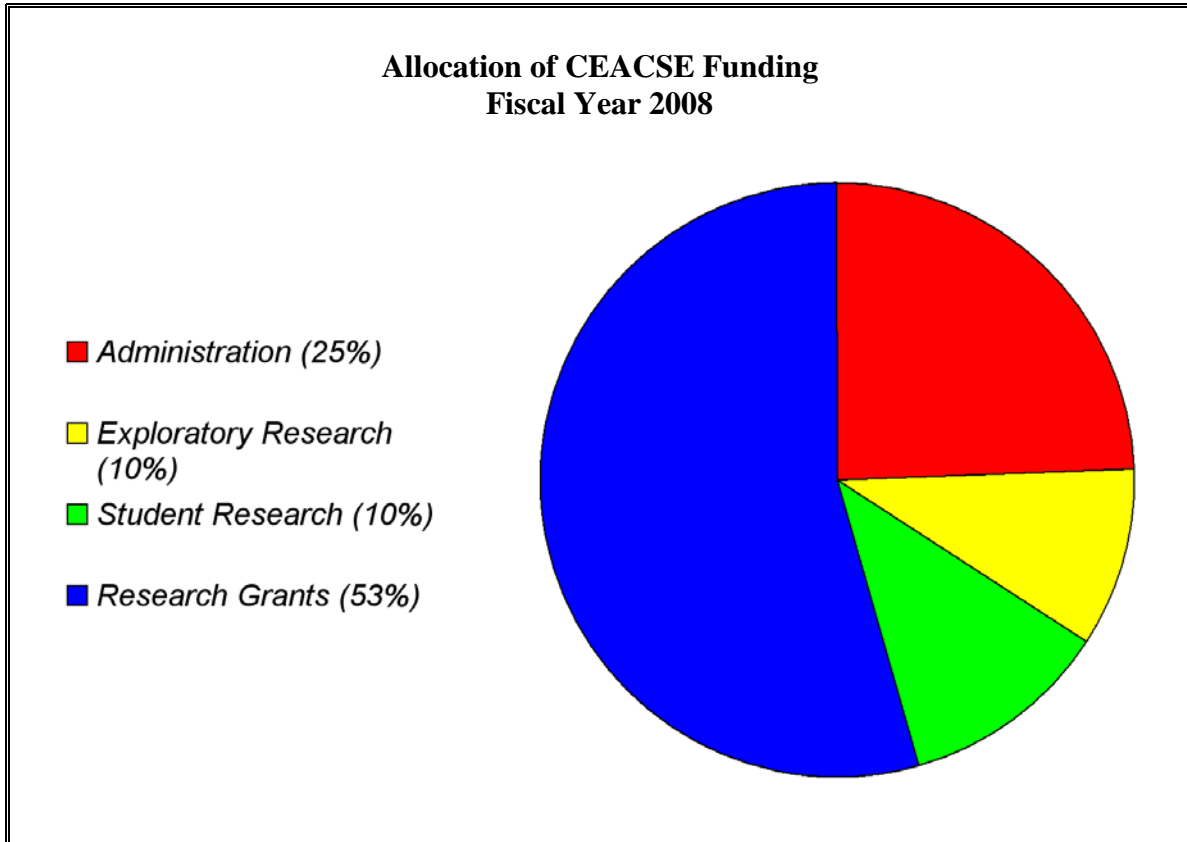
#### **15. Modeling and Analysis of Combustion Instability in Rocket Engines and Motors**

- Principal Investigator(s): Dr. Robert Webster, Graduate School of Computational Engineering
- Objective(s): To develop and demonstrate capability to analyze combustion chamber acoustic characteristics, physics of laminar diffusion flames, and their combined effects. To add higher-order schemes for improved accuracy into the flow solver(s) and to include sensitivity derivatives for effects of physical and design parameters.
- Seed Funding: \$106,600
- Results: Dr. Webster contributed to a proposal for external funding to ERC, Inc and the US Air Force Research Laboratory, and is awaiting award notification of \$150,000.

Total Seed Funding: \$ 927,600



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.



*Figure 2*

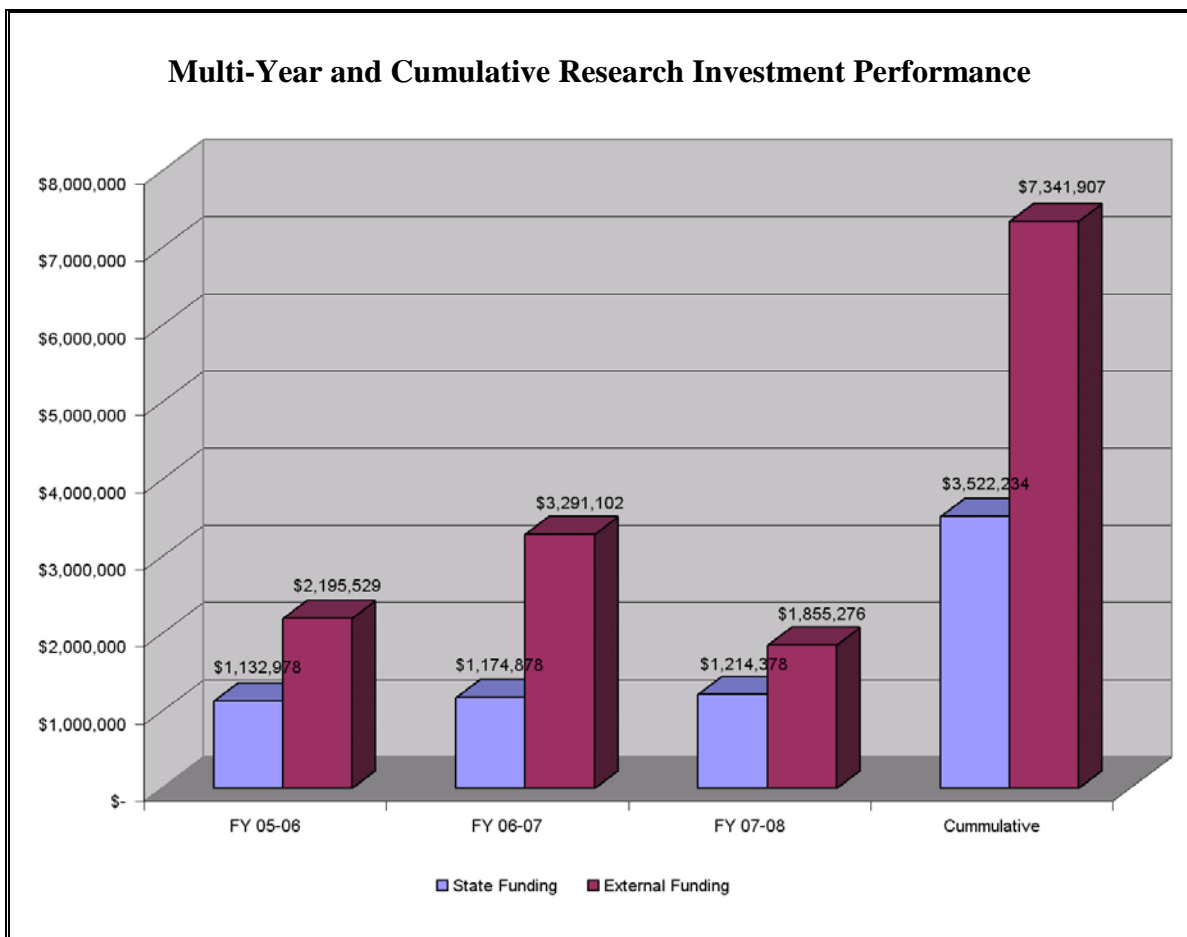
***External Funding Awarded as the Result of the Center’s Research Investment\****

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
<b>Total External Funding Awarded:</b>	<b>\$7,341,907</b>

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\* These funds represent funds committed by external funding agencies. Some of the awards included are multi-year awards with each year’s funding dependant 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 FY08. This performance has been consistent and CEACSE works toward continuous improvement.



*Figure 3*

*FY 2008 Publications and Presentations of the Center's Research Activities*

1. Cemerlic, A., Yang, L., Kizza, J.M., "Network Intrusion Detection Based on Bayesian Networks", Proceedings of Software Engineering and Knowledge Engineering (SEKE08), July 2008.
2. Hajjawi, M., Taylor, L., and Nichols, D. S., "Assessment and Modification for Reynolds Stress Transport Turbulence Model Flow Prediction", AIAA-2008-0568, 46th AIAA Aerospace Sciences Meeting and Exhibit, January 2008.
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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 UTC Center Center of Excellence in Applied Computational Science & Engineering

	FY 2007-08 Actual			FY 2008-09 Proposed			FY 2009-10 Requested		
	Matching	Appropri.	Total	Matching	Appropri.	Total	Matching	Appropri.	Total
	357,578	856,800	1,214,378	357,578	821,300	1,178,878	357,578	862,365	1,219,943
<b>Salaries</b>									
Faculty	188,982	462,681	651,664	223,035	479,878	702,913	193,092	465,677	658,769
Other Professional	25,583	62,634	88,217	27,991	60,226	88,217	25,857	62,360	88,217
Clerical/ Supporting	5,412	13,249	18,661	5,921	12,740	18,661	5,470	13,191	18,661
Assistantships	64,382	157,625	222,008	70,443	151,565	222,008	65,073	156,935	222,008
Total Salaries	284,359	696,190	980,549	327,390	704,409	1,031,799	289,492	698,163	987,655
Fringe Benefits	56,480	138,279	194,759	67,331	144,869	212,200	57,213	137,979	195,192
Total Personnel	340,839	834,469	1,175,308	394,721	849,278	1,243,999	346,705	836,142	1,182,847
<b>Non-Personnel</b>									
Travel	6,060	14,836	20,896	6,630	14,266	20,896	2,931	7,069	10,000
Software	83	202	285			0			0
Books & Journals	54	132	186	59	126	185	50	121	171
Other Supplies	783	1,918	2,701	842	1,810	2,652	586	1,414	2,000
Equipment			0			0			0
Maintenance			0			0			0
Scholarships	21,037	51,505	72,542	18,568	39,950	58,518	7,306	17,619	24,925
Consultants	5,800	14,200	20,000			0			0
Renovation			0			0			0
Other (Specify)			0			0			0
Communications	333	815	1,148			0			0
			0			0			0
			0			0			0
Total Non-Personnel	34,150	83,608	117,758	26,099	56,152	82,251	10,873	26,223	37,096
GRAND TOTAL	374,989	918,077	1,293,067	420,820	905,430	1,326,250	357,578	862,365	1,219,943
<b>Revenue</b>									
New State Appropriation		856,800	856,800		821,300	821,300		862,365	862,365
Carryover State Appropriation		146,407	146,407		84,130	84,130			0
New Matching Funds	357,578		357,578	357,578		357,578	357,578		357,578
Carryover from Previous Matching Funds	80,653		80,653	63,242		63,242			0
Total Revenue	438,231	1,002,207	1,440,438	420,820	905,430	1,326,250	357,578	862,365	1,219,943