# 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 2008-2009

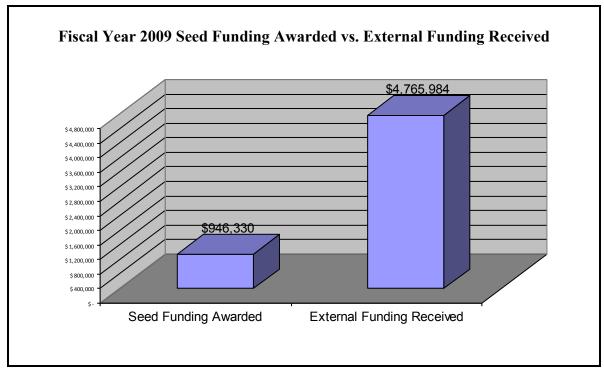
*September 28, 2009* 

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#### **Executive Summary**

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its fourth 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 issue is the necessity to grant time extensions to researchers who were awarded seed funding during the previous fiscal years. This is partially affected by current teaching demands. For the most part though the reporting year has proceeded smoothly with the majority of the awarded research funds being expended. This issue has improved with zero extensions granted for FY09.

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 exceeded a five 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, local companies are assisting in funding 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 stated in previous reports, as a result of funding research activities and secured external funding, several companies are and continue to operate 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 2009 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. 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 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.

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 & Table 2).

At the start of its fourth year, CEACSE granted funding to thirteen proposed research projects, and carried forward 2007-2008 funding for seven research projects. In addition, sixteen exploratory research activities were approved and funded during Fiscal Year 2009 (Table 3). 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. In general, these grants are small in nature and of limited duration and scope although there are exceptions on occasion. 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 1CEACSE Seed Funding Committed for FY 2008-2009 Research Activities

		One-Year		Proposal	Externally	
Project Title	Budget	Extension	Expenses	Submitted	Funded	External Funding Source(s)
						Office of Naval Research;
Computational Analysis and Design of Fuel Cell Components	\$15,059	Ν	\$5,293	Y	Y	\$3,354,350
Computational Simulation of an Experimental Kudsen Compressor	\$60,000	Ν	\$59,002	Ν	Ν	
Tenasi Performance Enhancement for Petascale Computing	\$49,665	Ν	\$42,982	Ν	Ν	
Agent based modeling (ABM) code to biological systems,						
transportation and risk management	\$14,000	Ν	\$14,192	Pending	Ν	
A panic model for the SimCenter Agent Based Modeling (ABM)						
code	\$34,000	N	\$33,284	Pending	N	
Agglomeration model for the Tenasi particle module	\$34,000	N	\$32,344	Y	Y	ERC, Inc./Air Force Research Lab \$150,000
TinyID: A Revolutionized Warehouse Management Tool	\$40,000	N	\$23,619	Y	Y	NSF CPS, \$469,000
Implementation of an arbitrary equation of state into the Tenasi						
family of flow solvers	\$40,865	Ν	\$39,122	Ν	Ν	
Improving the order of accuracy for unstructured flow solvers	\$53,158	Ν	\$52,781	Y	Pending	
Implementation of the phase field approach into the Tenasi						
unstructured solver	\$34,000	Ν	\$33,533	Ν	Ν	
Level Set Approach for Chemical Etching and Deposition	\$34,000	Ν	\$33,139	Ν	Ν	
Fluid-Structure Interaction for Ship Hydrodynamics	\$68,000	N	\$65,408	Ν	Ν	
A Fast Response and Planning System in Disaster Management	\$40,000	Ν	\$23,797	Y	Y	DoD Scholarship; \$26,080

Table 2CEACSE Seed Funding Carried Forward from FY 2007-2008 to FY 2008-2009 Research Activities

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Analysis and sensitivity derivatives for plasma simulation	\$33,722	Y	\$33,780	Y	Ν	
Simulation of Biodiesel Production by Microreaction Systems	\$7,203	Y	\$7203	Ν	Ν	
Analysis and improvements to component technologies for a robot design optimization solver	\$163,107	Y	\$78,667	Y	Y	Space and Missile Defense Command
Physical/Mathematical Modeling and Solution of Field Simulation Problems	\$18,195	Y	\$17,949	Y	Y	Space and Missile Defense Command
Atmospheric wind modeling for regional simulations	\$59,032	Y	\$52,370	Y	Pending	
Wall modeled large eddy simulation turbulence model (WMLES)	\$48,122	Y	\$47,090	Ν	Ν	
Combustion instability in high-pressure, high-temperature combustors	\$100,202	Y	\$91,299	Y	Y	ERC, Inc./Air Force Research La

**One-Year** Proposal Externally Budget Expenses Submitted Funded **External Funding Sour** Extension itle e Methodologies for Unstructured Grid Generation, \$6,608 s, and Adaptation Ν Ν Ν Dissipation Formulations for Highly vertical Flows and Ν \$37,908 Ν Ν e flows Liquid Rocket Propulsion Simulations Ν Ν Ν \$3,948 \$6,000 on of Porous Media Flows Ν Ν Ν Ν Ν Ν on of Agent Based Models for Urban Evacuations \$3.000 Ν Ν Ν Simulations \$5,000 ics/Multiregime Algorithm Formulation Ν \$5,000 Ν Ν Ν Ν Ν \$7,500 Fuel Cell Formulation is of Fluid Structure Interaction for Marine Vehicles Ν Ν Ν \$7,500 is of Embedded Propulsion Systems with Flow Control Ν \$1,250 Ν Ν tion of Applicability of Fuel Cell Modeling for Battery Ν \$6,000 Ν Ν Ν der spatial discinetization for Unstructured Grids Ν \$4,858 Ν is of ships in varying sea states Ν \$5,813 Ν Ν Ν on of vaporous hazardous material release and trajectory Ν \$5,000 Ν vine Simulations Ν \$1,250 Ν Ν Simulations Ν \$1,250 Ν Ν

 Table 3

 CEACSE Exploratory Research Activities for FY 2008-2009

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 22 faculty members from various disciplines, such as physics, computer science, and computational engineering, including one Masters level student who was also a staff member. CEACSE funding has continued the support of nine Ph.D. graduate students, nine Masters level graduate students, and eight undergraduate students. One previous Ph.D. student working under a grant graduated in August 2008 and is continuing in a research faculty position at the University. One Masters level student who worked on a grant graduated in August 2008 and is currently pursing his Ph.D. 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 four years, CEACSE faculty have made at least 110 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 contributes to and enables the following activities at the SimCenter that are supportive of economic development:

 A journal article will be 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 will appear in Computers and Fluids:

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", to appear in Computers and Fluids, 2009.

2. The SimCenter continues a close partnership with a Huntsville-based emerging technology firm, Radiance Technology, Inc., who now maintains a project office in Chattanooga with eight engineers. Radiance and the SimCenter have a government-sponsored research collaboration in electromagnetics. Radiance continues to utilize SimCenter faculty and UTC PhD graduates, and PhD. students. This is a significant event because the SimCenter partnership with Radiance has enabled new jobs that allow 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, which were completed, 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 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, although it is in an inactive state.

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. The center hosted 150 students from Tyner Middle, Normal Park Middle, Soddy-Daisy Middle, Central High School, Battle & Brown Elementary Schools, and a local Girls, Inc. group. 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. 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 highachieving 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. 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.

#### **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.

### Completed in Fiscal Year 2008-2009

## 1. Analysis and Sensitivity Derivatives for Plasma Simulations

- Principal Investigator(s): Dr. Kyle Anderson, Graduate School of Computational Engineering
- Objective(s): To continue developing computational methods for numerically simulating RF capacitive-coupled discharge plasmas, and to provide sensitivity analysis for obtaining better understanding of the underlying physics and for tailoring plasma processes using design procedures.
- Seed Funding: \$ \$76,732
- Results: A proposal was submitted to NSF but was not funded

## 2. Simulation of Biodiesel Production by Microreaction Systems

- Principal Investigator(s): Dr. Frank Jones, Chemical Engineering
- Objective(s): To program a micro processing plant to produce biodiesel fuel using CFD ACE+ commercial software. Many design variations will be examined, ultimately, the design group will fabricate and operate the most promising of these designs.
- Seed Funding: \$ 25,000
- Results: No proposals were submitted

## **3.** Analysis and Improvements to Component Technologies for a Robust Design Optimization Solver

- Principal Investigator(s): Dr. Chad Burdyshaw, Dr. Kyle Anderson, Graduate School of Computational Engineering
- Objective(s): To fund the research and development of methods to improve the capability and robustness of the existing design optimization software.
- Seed Funding: \$ 239,506
- Results: A proposal submitted to the Space and Missile Defense Command and was funded for \$1,261,598.

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

- Principal Investigator(s): Dr. Roger Briley, Dr. Dave Whitfield, 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 expertise can leveraged within these areas, and to link these opportunities to potential funding sources.
- Seed Funding: \$ 100,000

• Results: Proposal submitted to the Space and Missile Defense Command and was funded for \$1,261,598.

### 5. Atmospheric wind modeling for regional simulations

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering
- Objective(s): This effort focuses on the creation of a quasi-stochastic atmospheric model that will be dependent upon both advanced turbulence modeling and parameterized inputs to model variability of wind speed and direction, eddies, thermal effects, and ground cover.
- Seed Funding: \$ 118,625
- Results: A proposal was submitted to DOE for \$444,446 and is pending approval.

## 6. Hybrid Turbulence Models for Vortex and Separated Flows

- Principal Investigator(s): Dr. Lafayette Taylor, Graduate School of Computational Engineering
- Objective(s): To develop advanced hybrid turbulence models that can accurately predict massively separated and cortex dominated flows.
- Seed Funding: \$ 118,625
- Results: A proposal was submitted to ERC, Inc and was funded for \$150,000.

## 7. Combustion Instability in High-Pressure, High-Temperature Combustors

- Principal Investigator(s): Dr. Robert Webster, Graduate School of Computational Engineering
- Objective(s): To further develop and demonstrate the capability to analyze the fundamental processes, both individually and combined, that contribute to combustion instability.
- Seed Funding: \$ 177,891
- Results: A proposal was submitted to ERC, Inc and was funded for \$150,000.

## New Research Activities Funded by the Center in Fiscal Year 2008-2009

## 1. Computational Analysis and Design of Fuel Cell Components

- Principal Investigator(s): Dr. Kyle Anderson
- Objective(s): To continue the development of the simulation and design codes 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: \$ 15,059
- Results: A proposal was submitted to ONR and was funded for \$3,354,350.

#### 2. Computational Simulation of an Experimental Knudsen Compressor

- Principal Investigator(s): Dr. Glenn Brook, Graduate School of Computational Engineering
- Objective(s): To improve the performance of the Boltzmann-BGK solver in use at the SimCenter and apply the improved solver to the investigation of an experimental Knudsen compressor relative to actual device geometries.
- Seed Funding: \$60,000
- Results: No proposals were submitted.

#### 3. Tenasi Performance Enhancement for Petascale Computing

- Principal Investigator(s): Dr. Daniel Hyams, Graduate School of Computational Engineering
- Objective(s): To research and implement methods into the Tenasi code that address each of these barriers to high efficiency scalability to petascale computing levels
- Seed Funding: \$ 49,665
- Results: No proposals were submitted, although all externally funded projects utilizing Tenasi benefit from this work.

## 4. Extension of the SimCenter Agent Based Modeling Code to biological systems, transportation and risk management

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To study the feasibility of extending the SimCenter ABM system into the fields of biological, transportation and risk management.
- Seed Funding: \$ 14,000
- A proposal in collaboration with Brookings Institute will be submitted at a later time.

#### 5. A panic model for the SimCenter Agent Based Modeling code

- Principal Investigator(s): Dr. Ramesh Pankajakshan Graduate School of Computational Engineering
- Objective(s): To design, implement and validate a panic model for the SimCenter ABM code.
- Seed Funding: \$ 34,000
- Results: Proposals for funding further development and evaluation of ABM-CFD hybrid evacuation modeling of large cities will be submitted later in the year. A manuscript has been submitted to PNAS.

#### 6. An agglomeration model for the Tenasi particle module

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To implement a highly simplified agglomeration model which can produce post-contact particle populations with reasonable radius and velocity statistics. Both stochastic and deterministic collision models will be considered.
- Seed Funding: \$ 34,000
- Results: A proposal was submitted to ERC, Inc and was funded for \$150,000.

#### 7. TinyID: A Revolutionized Warehouse Management Tool

- Principal Investigator(s): Dr. Mina Sartipi, Computer Science and Engineering
- Objective(s): To maintain the accuracy and reliability of the TinyID system, and considering the cost and energy constraints on individual TinyID tags, by proposing and modifying the existent algorithms on : Efficient and flexible routing, network security and date aggregation.
- Seed Funding: \$ 40,000
- Results: Dr. Sartipi submitted proposals for external funding to:
  - i. NSF Career, Not funded.
  - ii. NSF BRIGE, Not funded
  - iii. NSF CPS, Funded for \$469,000
  - iv. Global Environment for Network Innovations, Not funded

## 8. Implementation of an arbitrary equation of state into the Tenasi family of flow solvers

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): To develop and implement an algorithm capable of numerically simulating a fluid with an arbitrary equate of state.
- Seed Funding: \$ 40,865
- Results: No proposals were submitted.

### 9. Improving the order of accuracy for unstructured flow solvers

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): To develop and implement approaches that will improve the order of accuracy of the unstructured flow solver.
- Seed Funding: \$ 53,158
- Results: A proposal was submitted to DOE for \$444,446 and is pending.

- 10. Implementation of the Phase Field Approach into the Tenasi Unstructured Solver
  - Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
  - Objective(s): To implement a phase field approach into the current Tenasi unstructured solver for tracking of multiphase gas/liquid and liquid/solid phase change interfaces.
  - Seed Funding: \$ 34,000
  - Results: No proposals were submitted.

### 11. Level set approach for chemical etching and deposition

- Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): To extend the current Tenasi unstructured level set fabrication of electronic devices during etching and deposition processes.
- Seed Funding: \$34,000
- Results: No proposals were submitted.

## 12. Fluid-Structure interaction for ship hydrodynamics

- Principal Investigator(s): Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): To develop and use a relatively straightforward ID Euler-Bernoulli or Timoshenko beam equation solver to model the unsteady structural response of a surface ship to incident waves.
- Seed Funding: \$68,000
- Results: No proposals were submitted.

## 13. A Fast Response and Planning System in Disaster Management

- Principal Investigator(s): Dr. Li Yang, Computer Science and Engineering
- Objective(s): To provide a platform for different emergency responding teams to communicate and collaborate with each other, integrate intelligence and information, and deploy real-time and effective emergency strategies using situational data and existing knowledge base.
- Seed Funding: \$40,000
- Results: Dr. Yang submitted proposals for external funding to:
  - i. Restructure Cryptography Curriculum, NSF CCLI, Not funded.
  - ii. Developing a Prototype to Secure Collaboration in GENI and Educating Students using GENI, NSF GENI Solicitation, Not funded
  - UTC Information Assurance Scholarships and Capacity Building Program. Department of Defense. Scholarship: Partially awarded for \$26,080

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.

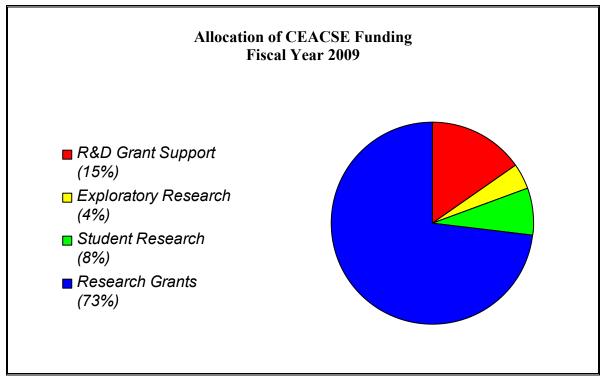


Figure 2

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

Total External Funding Awarded:	\$12,107,891
External Funding Awarded in Fiscal Year 2008-2009:	\$ 4,765,984
External Funding Awarded in Fiscal Year 2007-2008:	\$ 1,855,276
External Funding Awarded in Fiscal Year 2006-2007:	\$ 3,291,102
External Funding Awarded in Fiscal Year 2005-2006:	\$ 2,195,529

<sup>\*</sup> 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 cumulative outcome from funding provided to CEACSE by The State of Tennessee and The University of Tennessee at Chattanooga illustrates the achievement of nearly 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 FY09. This performance has been consistent and CEACSE works toward continuous improvement.

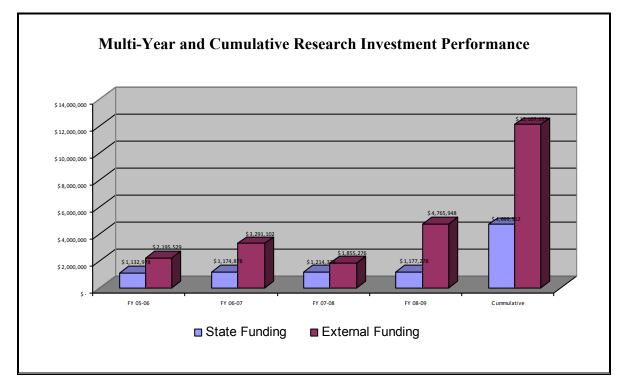


Figure 3

#### FY 2009 Publications and Presentations of the Center's Research Activities

- 1. <u>Applied Cryptography for Cyber Security and Defense: Information Encryption and Cyphering</u>, Hamid R. Nemati and Li Yang (editors), *in progress*.
- 2. Harkeerate Bedi, Li Yang, Joseph Kizza, Biometrics based Fair Electronic Exchange, *the Proceedings of Cyber Security and Information Intelligence Research Workshop*, ACM Digital Library, Oak Ridge, TN, April 2009
- 3. Li Yang, Alma Cemerlic, Integrating Dirichlet Reputation into Usage Control, *the Proceedings of Cyber Security and Information Intelligence Research Workshop*, ACM Digital Library, Oak Ridge, TN April 2009
- 4. Li Yang, Lu Peng, and Balachandran Ramadass, SecCMP: Enhancing Critical Secrets Protection in Chip-Multiprocessors, *International Journal of Information Security and Privacy*, Volume 2, Issue 4, pp. 54-66, October-December 2008.
- 5. Li Yang, Feiqiong Liu, Joseph M. Kizza, Raimund K.Ege. Discovering Latent Topics from Dark Websites, IEEE Symposium on Computational Intelligence in Cyber Security, IEEE Xplore, Nashville, TN, March 2009.
- 6. Ran Tao, Li Yang, Lu Peng, Bin Li, Alma Cemerlic. DoS Network Intrusion Detection through Multi-layer Features, IEEE Symposium on Computational Intelligence in Cyber Security, IEEE Xplore, Nashville, TN, March 2009.
- 7. Raimund K. Ege, Li Yang, and Richard Whittaker, Proceedings of The Fourth International Conference on Systems, IEEE Xplore, France, March 2009.
- 8. Li Yang, Teaching Database Security and Auditing, Proceedings of the 40th ACM Technical Symposium on Computer Science Education (SIGCSE), Chattanooga TN, March 2009.
- 9. Sivakumar, P., Hyams, D.G., Taylor, L.K., and Briley, W.R., "Primitive-Variable Riemann Fluxes for Solution of the Shallow Water Equations with Embedded Wet/Dry Interfaces," UTC-CECS-SimCenter-2008-06, November 2008.
- Wilson, R., Lei, J., Karman, Jr., S., Hyams, D., Sreenivas, K., Taylor, L., and Whitfield D., 2008, "Simulation of Large Amplitude Ship Motions for Prediction of Fluid-Structure Interaction," Proceedings of the 27th ONR Symposium on Naval Hydrodynamics, Seoul, Korea, 5-10 Oct. 2008.
- Karman, Jr., S. L., and Wilson, R., 2008, "Hierarchical Unstructured Mesh Generation with General Cutting for Free Surface Simulations," Proceedings of the 27th ONR Symposium on Naval Hydrodynamics, Seoul, Korea, 5-10 Oct. 2008.

- Lee, D., Maki, K., Wilson, R., Troesch, A., and Vlahopoulos, N., Dynamic Response of a Marine Vessel Due to Wave-Induced Slamming, Int. Sym. On Vibro-Impact Dynamics of Ocean Systems and Related Problems, Troy, Michigan, 2-3 Oct. 2008.
- 13. Lange, K. and Anderson, W.K. "Using Sensitivity Derivatives for Design and Computing Error Bounds in an Atmospheric Plasma Discharge Simulation." 61st Annual Gaseous Electronics Conference, October 2008.
- 14. Briley, W. Roger and McDonald, H., "Reflections on the Evolution of Implicit Navier-Stokes Algorithms," UTC-CECS-SimCenter-2008-04, September 2008.
- 15. Wilson, Robert V., "A Review of Computational Ship Hydrodynamics," UTC-CECS-SimCenter-2008-03, September 2008.
- 16. Anderson, W. Kyle, Karman, Steve L., and Burdyshaw, Chad, "Geometry Parameterization Using Control Grids," AIAA 2008-Presented at the 12th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, Victoria, BC, September 10-12, 2008.
- Lange, K. and Anderson, W.K. "Sensitivity Derivatives for Plasma Discharge Simulations." AIAA-2008-5930. 12th AIAA/ISSMO Multidisciplinary Analysis and Optimization Conference, September 2008.
- Sahasrabudhe, M., "Unstructured Mesh Generation and Manipulation based on Elliptic smoothing and Optimization," Ph.D. Dissertation, University of Tennessee at Chattanooga, August 2008.
- 19. Sivakumar, P., Hyams, D.G., Taylor, L.K., and W.R. Briley, "A Primitive-Variable Riemann Method for Solution of the Shallow-Water Equations with Wetting and Drying," Journal of Computational Physics, Vol. 228, No.19, pp. 7452-7472, 2009.
- 20. Sreenivas, K., Taylor, Lafayette K., Briley, W. Roger, "Unsteady Flow Simulations for an Aerotonomy-Designed Synthetic-Jet Airfoil," UTC-CECS-SimCenter-2009-02-R, June 2009.
- 21. Kapadia, S., Anderson, W. K., and Burdyshaw, C., "Channel Shape Design of Solid Oxide Fuel Cells," UTC-CECS-SimCenter-2009-01, June 2009.
- 22. Dweik, Z., Briley, W.R., Swafford, T.W., and Hunt, B., "Computational Study of the Heat Transfer of the Buoyancy-Driven Rotating Cavity with Axial Throughflow of Cooling Air," GT2009-59978, ASME Turbo EXPO 2009, June 8-12, 2009, Orlando, FL.

- 23. Dweik, Z., Briley, W.R., Swafford, T.W., and Hunt, B., "Computational Study of the Unsteady Flow Structure of the Buoyancy-Driven Rotating Cavity with Axial Throughflow of Cooling Air," GT2009-59969, ASME Turbo EXPO 2009, June 8-12, 2009, Orlando, FL.
- Anderson, W.K., Karman, S.L., and Burdyshaw, C., "Geometry Parameterization Method for Multidisciplinary Applications," AIAA Journal, Vol. 47, No. 6, June 2009.
- 25. Chen, J-P, Johnson, B., Hathaway, M.D., and Webster, R.S., "Flow Characteristics of Tip Injection on Compressor Rotating Spike via Time-Accurate Simulation", Journal of Propulsion and Power, Vol. 25, No. 3, May-June, 2009, pp. 678-687.
- Boelens, O.J., Badcock, K.J., Görtz, S., Morton, S., Fritz, W., Karman, S.L., Michal, T., and Lamar, J.E., "F-16XL Geometry and Computational Grids Used in Cranked Arrow Wing Aerodynamics Project International," *Journal of Aircraft*, Vol. 46, No. 2, March–April 2009, pp. 369-376.
- Kapadia, S. and Anderson, W.K., "Sensitivity Analysis for Solid Oxide Fuel cells using a Three-Dimensional Numerical Model," *Journal of Power Sources*, Volume 189, Issue 2, April, 2009, Pages 1074-1082
- Kapadia, S., Anderson, W.K., Elliott, L., Burdyshaw, C., "Adjoint-Based Sensitivity Analysis and Error Correction Methods Applied to Solid Oxide Fuel Cells." (To be published in ASME Journal of Fuel Cell Science and Technology)
- 29. Karman, S. L. and Sahasrabudhe, M., "Unstructured Elliptic Smoothing Revisited", 47th Aerospace Sciences Meeting and Exhibit, January 5th - January 9th, 2009, Orlando, Florida, AIAA-2009-1362.

#### **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 precollege 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

UT Chattanooga FY 2008-09 Actual FY 2009-10 Proposed FY 2010-11 Requested Matching Matching Matching Appropr. Total Total Total Appropr. Appropr. 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 ongevity 104 244 348 161 339 500 178 422 600 179,700 Fringe Benefits 53.910 125,790 92.493 194.753 287,246 77.978 185.462 263,440 1,034,421 Total Personnel 310.326 724.095 414.332 872.414 1.286.746 340.708 810,332 1,151,040 Non-Personnel 6,143 14,334 7,084 14,916 5,920 14,080 Travel 20,478 22,000 20,000 1,500 3,500 5,000 483 1,017 1,500 1,056 Software 444 1,500 19 51 75 22 53 Books & Journals 45 24 75 64 15 35 Other Supplies 51 354 746 1,100 355 845 1,200 Equipment 0 0 0 Maintenance C 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 819,700 819,700 811,200 811,200 851,760 851,760 Appropriation Carryover State 84,130 84,130 126,335 126,335 Appropriation ( New Matching Funds Carryover from Previou 357,578 357,578 357,578 357,578 357,578 357,578 Matching Funds 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

Center

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