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 2011-2012**

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Executive Summary

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its seventh year of operation. The previous years have led to the establishment and development of an effective operation. This period has provided an opportunity 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 continues operation. One 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 and continuing increase in the number of students in classes by those sought to provide research proposals. There are continuing issues as well, the national economic environment, level of external funding committed to research and development funding, and increased externally competitive environment. The reporting year has proceeded smoothly with the awarded research funds being expended.

As is noted in this report, CEACSE continues to accomplish its mission and objectives. Through the awards, the researchers and associated academic units have maintained external funding from various agencies, companies, and governmental entities. CEACSE monies from the 2012 fiscal year as well as from past years continue to provide returns, reaping benefits through additional awards/grants. (Figure 1).
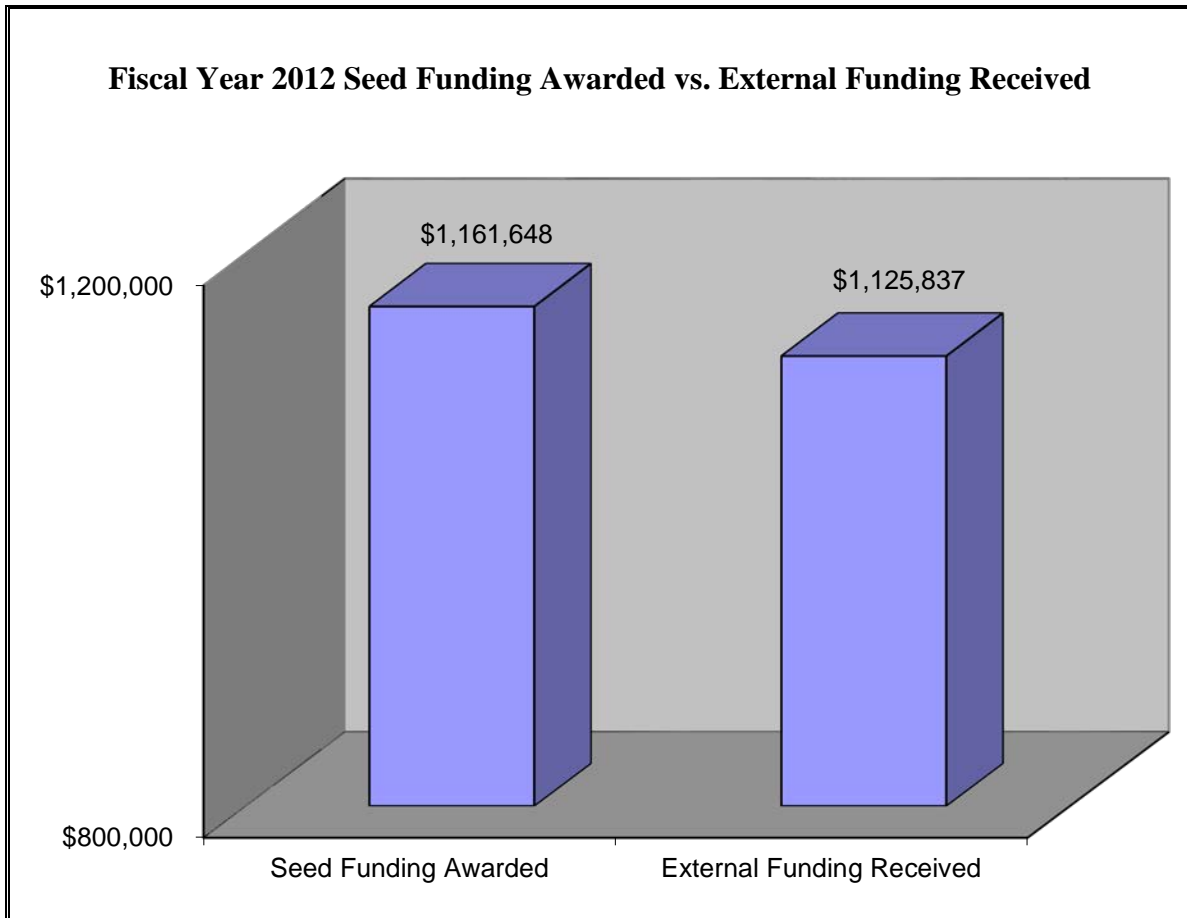
Fiscal Year 2012 Seed Funding Awarded vs. External Funding Received

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. There is a continuing reach to both graduate and undergraduate students and they have participated on various research activities undertaken as a result of CEACSE funding. Due to the research activities that some of the students have undertaken, local companies continue to have interest in the student's educational programs impacted by the CEACSE research. The SimCenter: National Center for Computational Engineering continues to be a research anchor and attract students locally as well as nationally and internationally.

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

The following is the Annual Report for Fiscal Year 2012 of CEACSE activities and efforts.

Introduction

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

Center Research Focus

CEACSE is strategically focused on synergistic new programs that will collectively advance the state of the art in computational simulation in solving complex problems in the physical sciences and engineering that require and utilize scientific supercomputing. This focus encompasses research on computational simulations for analysis of the physical processes embedded in real 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. The ranking of the SimCenter cluster has been enhanced from the previous years. Meanwhile, other organizations and universities around the world continue to upgrade their equipment, presenting continuing increased need for computing capability. With additional funding, the SimCenter could stay competitive and once again rank among the Top 500.

The utilization of available cluster-supercomputer resources for appropriate and promising research projects is of considerable importance.   A ranking of a computing machine is a measure of raw computing power, but it does not ensure that the research undertaken is itself worthwhile or that the computed results produced are significant. The intellectual and practical value of each specific research project is the primary objective, and the computer itself serves as the enabling resource.

There has been an ongoing expansion of capabilities to broaden research and support activities. The Center requires that at least one external proposal be developed for each seed funded activity and submitted to a funding agency for continuation and expansion of the CEACSE funded research or related research. During this most recent year of operation it can be seen that the

Center's funded activities and philosophies are continuing to achieve results

(Table 1).

At the start of its seventh year, CEACSE granted funding to nineteen proposed research projects.   In addition, several exploratory research activities were approved and funded during Fiscal Year 2012 (Table 2). The exploratory research activities included research performed in support of requests received from external funding agencies, efforts to find external funding opportunities for a number of the CEACSE funded projects, white paper and proposal preparation assistance, and research activities undertaken by the Center's Staff. As a result, several of these opportunities have been identified throughout the course of the fiscal year. One such example of exploratory research activities is environmental component modeling The activities

arise throughout the year and thus fall outside the standard award cycle. These exploratory activities are evolving as increasingly important components of research activities. These are needed to respond increasingly to frequent demands to the new complex evolving problems. Consequently, these research activities were initiated at the discretion of the Center's Director. 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 2011-2012 Research Activities

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Tetrahedral Mesh Creation /Optimization Using Edge/Face Flips	$44,700	N	$44,627	N	N	
Investigation of Local Low Mach Number Preconditioning Schemes	$46,127	N	$46,127	N	N	
Physics-Based Modeling for Multi-material Interfaces	$46,127	N	$45,853	Y	Y	Shaw Industries, $5,949
Extended Capabilities for Electromagnetic Simulations	$149,502	Y	$144,560	N	N	
Numerical Simulation of Lithium-Ion Batteries	$100,467	Y	$99,289	N	N	
Navier-Stokes Utilizing Discontinuous Galerkin/Petrov Galerkin Approaches	$100,476	Y	$98,906	Y	Decision Pending	AFSOR, $359,523, awaiting decision; NSF, $408,186 awaiting decision
LES of Chemically Reacting Flows	$69,877	N	$69,877	N	N	
Direct Numerical Simulation (DNS) for a Priori Large-Eddy Simulation (LES) Sub-grid Model Evaluation	$69,877	N	$69,318	N	N	
Development of an Overset Grid Approach for the Tenasi Code Flow Solver	$52,800	N	$52,800	N	N	
Multi-Regime Solution Capability via Ghost-Fluid Method	$52,800	N	$52,357	N	N	
Shape and Topology Optimization using the UT-Tenasi Code	$50,670	N	$49,577	N	N	
Numerical Simulation of Respiratory Flow Patterns within Human Lung	$53,852	N	$46,217	N	N	
Development and Verification of an Analytical Wake Model for Wind Farm Op	$30,000	N	30,000	Y	Y	NSF, $283,209
Applications of SimCenter Hybrid RANS/LES Code	$80,000	N	$80,000	N	N	
A Validation Study of Tenasi's Conjugate Heat Transfer	$70,235	N	$69,793	N	N	
Analysis and Design of Biological Stent Implants	$20,000	N	$19,625	Y	Decision pending	NIH, $300Awaiting decision from NIH
Enhanced Compression in Distributed Sensing Application	$40,000	N	$36,965	Y	N	
Online Opinion Mining on Social Media	$64,170	N	$62,230	Y	Y	NSF, $100,000; NSF, $382,528; NSF, $209,000 awaiting decision
Large-Scale Medical Image Modeling for Intelligent Medical Information Retrieval	$43,540	N	$40,032	Y	Y	NSF, $360,100, NSF, $305,494, recommended for funding; NSF, $213,497 awaiting decision
Tenasi Cloud Computing Initiative	33,576	N	$32,928	N	N	

Table 2
CEACSE Exploratory Research Activities for FY 2011-2012

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
River Flows	$14,094	N	$14,094	N	N	
Tenasi for Atmospheric Simulation	$23,955	N	$23,955	N	N	
Environmental Wind & Water Codes	$16,898	N	$16,898	N	N	
Robust Sensitivity Analysis	$24,530	N	$24,530	N	N	
Higher Order Atmospheric Reacting Flows	$5,556	N	$5,556	N	N	
Improving Run Time Efficiency of Tenasi	$14,869	N	$14,869	N	N	
Higher-Order Environmental Wind Flows	$9,064	N	$9,064	N	N	
Conjugate Heat Transfer	$17,264	N	$17,264	N	N	
Take-Off Simulation	$16,488	N	$16,488	N	N	
Hydrodynamic Fluid-Structure Interaction	$17,694	N	$17,694	N	N	
Disaster Mitigation	$14,278	N	$14,278	N	N	
Mesh Adaptation Library	$6,387	N	$6,387	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 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,

CEACSE funding has continued the support of seventeen Ph.D. graduate students, twelve Masters level graduate students, and seven undergraduate students. Three Masters level students who worked on a grant graduated in FY12 and are currently

pursuing their Ph.D. at the University of Tennessee at Chattanooga.   One Masters

level student who graduated in FY12 is pursuing his Ph.D. part time and is employed

with SimCenter Enterprises. 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 seven years, CEACSE faculty

have made at least 418 presentations during meetings for discussions directly related

to metropolitan engagement for the purpose of economic development, support of

local businesses and government, and planning for SimCenter expansion. Some

notable discussions pertaining to research opportunities occurred during this reporting

period with Shaw Industries, Inc., United Enertech and Global Green Lighting.

Research issues discussed included reduced power consumption, water penetration of

louvers, and heat transfer. 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. As energy costs continue to rise, industries search for areas in their
   manufacturing processes where they can reduce energy usage. If unfinished
   porous products are saturated with water one way to remove as much of the
   water as possible is through a simple vacuum extraction process. Many trial
   and error procedures have been attempted at Shaw Industries, Inc., however
   the energy consumed in this process is still extremely high. The discussions
   centered around the capability to model water extraction through a porous
   material that could be applied to this problem to try to maximize the amount
   of water extracted while minimizing the total energy consumed.

2. Under normal circumstances water does not penetrate an operating exhaust
   fan louver. However, in extreme wind driven rain events this typically is not
   the case. According to United Entertech, most customers purchase these
   louvers based on a rain penetration rating that is certified by a national testing
   organization. Discussions included the capability to simulate the certification
   procedure, which could lead to the improvement of the rain penetration
   performance of existing louvers.

3. Exposure to extreme heat shortens the life of LED lights. Global Green
   Lighting, a leader in the manufacturing and deployment of LED lighting
   devices, has determined that passive ventilation devices are preferred to active

devices (such as fans) due to powering requirements, failure rates, and

maintenance issues. Various passive ventilation and heat extraction strategies

to minimize temperatures near the LED lights could be investigated that

would extend the lifetime of the LED light.

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 and also partnered with other departments on campus. This year, the center has hosted over 800 students from Silverdale, Brown Middle School, Woodmore Elementary, Sequatchie County Middle School and Ooltewah High School. Several group activities were conducted, with culminating events such as a paper airplane design fly-offs, wind tunnel testing of a model airfoil, and concrete fracture testing (which the kids loved, as they got to break the samples). 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. With partnerships that are being forged with many local schools and organizations (i.e., we have a seat on the UTC Partnership Task Force, the CGLA Stem Board and a member of the curriculum for the new STEM school and hub being developed at Chattanooga

State), more contact time, better partnerships, and thus more depth and breadth 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. Seven 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) and a teaching presence in the undergraduate design and solid modeling classes has already gone a long way in spurring interest.

In March 2012, Vince Betro, our STEM Coordinator, accepted a position at ONRL. It was clear that Vince had made an impact on these individuals and demonstrated the SimCenter's efforts in this endeavor were worth the investment. As such we felt compelled to initiate a search for Vince's replacement. The search concluded in June 2012 with the hiring of Ms. Lindsey Frost as the new SimCenter STEM Coordinator. Lindsey is a 2009 economics graduate of Columbia University and began her career in STEM education with the Toshiba America Foundation in New York City. She comes to us from the Public Education Foundation (PEF) here in Chattanooga where she helped recruit, develop, and support Hamilton County's next generation secondary math and science teachers. Her work with the PEF enabled her to build strong relationships with local schools and various nonprofit organizations, which collectively will strengthen her efforts in SimCenter-related STEM activities. Lindsey will be working very closely with Julie Sanders who serves in a similar role with UTC's College of Engineering and Computer Science, to better coordinate and expand the College's and the SimCenter's promotion of STEM-related activities in the region. We are convinced Lindsey will be a major contributor; she is personable, professional, and well positioned to seek external funding to sustain STEM

activities over the long term, and most importantly, has a genuine passion for promoting STEM in local and regional schools.

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. **Tetrahedral Mesh Creation/Optimization Using Edge/Face Flips**
   - Principal Investigator(s): Mr. C. Bruce Hilbert, Graduate School of Computational Engineering
   - Objective(s): Continue the development of a tetrahedral mesh creation procedure using point insertion combined with edge and face flips to optimize the mesh quality.
   - Seed Funding: $44,700
   - Results: Development and testing complete. Further research is needed to increase speed and efficiency and also for a robust point insertion algorithm.

2. **Investigation of Local Low Mach Number Preconditioning Schemes**
   - Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
   - Objective(s): To explore preconditioning schemes (applied to the compressible flow equations) in order to assess their applicability and efficiency for practical problems of interest to the SimCenter. Also of interest would be time-accuracy and how best to achieve it using these local preconditioning schemes.
   - Seed Funding: $46,127
   - Results: Development continuing. Several schemes implemented and validated. Time accurate results still not satisfactory.

3. **Physics-Based Modeling for Multi-Material Interfaces**
   - Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
   - Objective(s): To explore physics-based modeling approaches for problems involving multi-material interfaces. These methods will be developed and tested for two-dimensional model problems with an eye on extending and implementing them for three-dimensional problems.
   - Seed Funding: $46,127
   - Results: Initial implementation and testing completed. Proposal submitted to Shaw in the amount of $5,949 and awarded. Further development needed to incorporate modeling of other multi-material interfaces.

4. **Extended Capabilities for Electromagnetic Simulation**
   - Principal Investigator(s): Drs. Kyle Anderson & Li Wang, Graduate School of Computational Engineering
   - Objective(s): To continue the development of high-order accurate (p>1) finite-element methods for electromagnetic simulations.
   - Seed Funding: $149,502

- Results: Development continuing to incorporate new capabilities, for inclusion in proposals including frequency-dependent materials.

5. **Numerical Simulation of Lithium-Ion Batteries**
   - **P**rincipal Investigator(s): Drs. Kyle Anderson & Sagar Kapadia, Graduate School of Computational Engineering
   - Objective(s): To develop computational methods for simulating lithium-ion batteries. Sensitivity derivatives will also be obtained for examining effects of physical parameters.
   - Seed Funding: $100,467
   - Results: Development complete and validated for one-dimensional simulations. Development continuing for three-dimensional simulations for inclusion in proposals.

6. **Navier-Stokes Utilizing Discontinuous Galerkin/Petrov Galerkin Approaches**
   - **P**rincipal Investigator(s): Drs. Kyle Anderson & Li Wang, Graduate School of Computational Engineering
   - Objective(s): To continue the development of higher-order accurate (p>1) discontinuous Galerkin (DG) and Petrov-Galerkin (PG) methods for delivering high-accuracy solutions of the Navier-Stokes equations. The emphasis for this project is to extend these capabilities for turbulent flow and to investigate the use of higher-order methods for large eddy simulations (LES).
   - Seed Funding: $100,476
   - Results:
   - Technology developed and demonstrated. Proposal submitted to AFOSR for $359,523 and is still pending; Proposal submitted to TN-SCORE for $50,000 which was not selected for funding; Proposal submitted to NSF for $408,186 and is still pending; Proposal submitted to NASA Langley for $594,858 was not selected for funding.

7. **LES of Chemically Reacting Flows**
   - Principal Investigator(s): Dr. Lafayette Taylor, Graduate School of Computational Engineering
   - Objective(s): Investigate the use and extension of LES techniques to compressible flow. Investigate LES as applied to high-speed external flows in which dissociation reactions can become relevant.
   - Seed Funding: $69,877
- Results: Implementation testing and validation of a LES model complete. Ready for use in application areas.

8. **Direct Numerical Simulation (DNS) for a Priori Large-Eddy Simulation (LES) Sub-grid Model Evaluation**
   - Principal Investigator(s): Dr. Lafayette Taylor, Graduate School of Computational Engineering

- Objective(s): Investigate the use of DNS as a means of evaluating present LES SGS models using a circular air jet discharging into quiescent air with the associated turbulent free shear layer. If possible, enhance present SGS models or develop new ones based on the DNS results.
- Seed Funding: $69,877
- Results: Partial validation of a LES model with DNS data complete.

New Research Activities Funded by the Center in Fiscal Year 2011-2012

1. **Development of an Overset Grid Approach for the Tenasi Flow Solver**
   - Principal Investigator(s): Drs. Kidambi Sreenivas & Robert Wilson, Graduate School of Computational Engineering
   - Objective(s): To initiate development of an in-house overset grid approach for the Tenasi unstructured flow solver. This initial phase will provide a proof concept, which can be further developed into a general overset capability for the Tenasi flow solver.
   - Seed Funding: $52,800
   - Results: Initial development and testing completed for simplified model. More development necessary for practical application.

2. **Multi-Regime Solution Capability via Ghost-Fluid Method**
   - Principal Investigator(s): Drs. Kidambi Sreenivas & Robert Wilson, Graduate School of Computational Engineering
   - Objective(s): To develop capability for solution of flows containing multiple regimes separated by material interfaces. The evolution of the material interface will be captured using the level set approach and appropriate jump conditions are enforced across the interface using ghost points.
   - Seed Funding: $52,800
   - Results: Development and initial testing completed. More physically realistic boundary condition development and implementation needed for practical applications.

3. **Shape and Topology Optimization using the UT-Tenasi Code**
   - Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering

- Objective(s): To add a shape and topology optimization capability to the existing sensitivity derivative module in the UT-Tenasi flow code.
- Seed Funding: $50,670
- Results: Methodology implemented and tested. Strategies to obtain the global optimum with reduced computational cost needs to be investigated.

4. Numerical Simulation of Respiratory Flow Patterns within Human Lung

- Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
- Objective(s): To access the current capability of the flow solver when applied to a bifurcating valve flow problem and enhance the capability of the solver to simulate flow representative of the internal flow of human lung airways.
- Seed Funding: $53,852
- Results: Initial testing on simplified geometries complete. Development continuing for more realistic geometries.

5. Development and Verification of an Analytical Wake Model for Wind Farm Op

- Principal Investigator(s): Dr. Lafayette Taylor, Graduate School of Computational Engineering
- Objective(s): Develop a methodology where a low fidelity optimization model will be used to get an optimum layout of a wind farm based on an analytical wake model. This optimum layout will be used as an initial solution for the high fidelity model with adjoint-based optimization to improve the layout.
- Seed Funding: $30,000
- Results: Proposal submitted to NSF and funded for $283,209.; Concept paper submitted to DOE was not selected for full proposal.

6. Applications of SimCenter Hybrid RANS/LES Code

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering
- Objective(s): The overall objective of the project is to demonstrate the new capabilities of the extended Tenasi code to potential clients in the helicopter industry and in the Homeland Security Agency.
- Seed Funding: $80,000
- Results: Development and implementation complete. Testing included rotorcraft and urban atmospheric dispersion.

7. A Validation Study of Tenasi's Conjugate Heat Transfer

- Principal Investigator(s): Dr. Robert Webster, Graduate School of Computational Engineering

- Objective(s): To validate existing technology for the treatment of conjugate heat transfer problems within the Tenasi software suite by conducting simulations of a variety of problems involving thermal-fluid coupling and making comparisons of the results with experimental data or purely theoretical solutions if available.
- Seed Funding: $70,235
- Results: Initial and continued testing uncovered difficulties with simulating these problem types. Other approaches to alleviate these short comings are being investigated.

8. **Analysis and Design of Biological Stent Implants**
   - Principal Investigator(s): Dr. Steve Karman, Graduate School of Computational Engineering
   - Objective(s): The project will focus the effects of fluid environment on the performance of implanted stents. The effects of plaque transport and attachment to artery walls are equally important. The project will use the SimCenter Tenasi code to compute the time accurate pulsed solution within a large straight natural artery, and a large straight stented artery. It will then use SimCenter design capability to improve stent performance.
   - Seed Funding: $20,000
     Results: Technology developed and demonstrated. Proposal submitted to NIH for $300,000 and is still pending.

9. **Enhanced Compression in Distributed Sensing Applications**
   - Principal Investigator(s): Dr.Mina Sartipi, Computer Science and Engineering
   - Objective(s): The goal is to design an algorithm that monitors temporal and spatial changes in the sensor readings in real time. For this purpose, we propose a data acquisition technique that not only exploits the sparsity of the signal, but also its pattern. The integration of these properties of the signals read by sensors can significantly improve the process of data acquisition in WSNs.
   - Seed Funding: $40,000
   - Results: Proposal submitted to NIH for $384,189 which was not funded. Proposal submitted to NSF for $416,232 which was not funded. Proposal submitted to NSF for $521,051 which was not funded.

10. **Online Opinion Mining on Social Media**
    - Principal Investigator(s): Dr. Li Yang, Computer Science and Engineering
    - Objective(s): Develop an automatic tool to analyze public opinion in non-western countries. Analyze casual and temporal relationship between the public sentiment and the real-world events. Model the Arabic "Internet opinion" and relate with the physical world protests. Understand how to

spread influence and interact with the public through social network and media.

- Seed Funding: $64,170
- Results: Proposal submitted to NSF for $100,000 and was funded; Proposal submitted to NSF for $382,528 and was funded; Proposal submitted to NSF for $209,000 and is still pending; Proposal submitted to DoD for $461,511 and is still pending; Proposal submitted to NSF for $554,779 and was not funded; Proposal submitted to NSF for $200,000 which was not funded.

11. Large-Scale Medical Image Modeling for Intelligent Medical Information Retrieval

- Principal Investigator(s): Dr. Yu Cao, Computer Science and Engineering
- Objective(s): Research, develop, evaluate and demonstrate a data-intensive and scalable intelligent medical image modeling and retrieval system with the capacity of finding the most clinically relevant images in response to specific information needs represented as search queries.
- Seed Funding: $64,170
- Results: Proposal submitted to NSF for $360,100 which was funded; Proposal submitted to NSF for $305,494 which was recommended for funding; Proposal submitted to NSF for $213,497 and is still pending; Proposal submitted to NSF for $123,376 which was declined for funding; Proposal submitted to NSF for $521,051 which was declined for funding.

12. Tenasi Cloud Computing Initiative

- Principal Investigator(s): Dr. Daniel Hyams, Graduate School of Computational Engineering
- Objective(s): Port Tenasi to a cloud computing environment for on-demand computations. Further, the Tenasi software suite and tools are to be modified such that cloud resources can be used just as easily as local computational resources.
- Seed Funding: $33,576
- Results: Development complete and capability validated. GUI ready for use if required.

Summary of CEACSE funding allocation (Figure 2) illustrates the major categories into which the CEACSE budget was allocated for Center activities during the past fiscal year of operation. It should be noted that grant awards from proposals and funding requests sought from this fiscal year funded projects normally will lag 6 to 12 months.
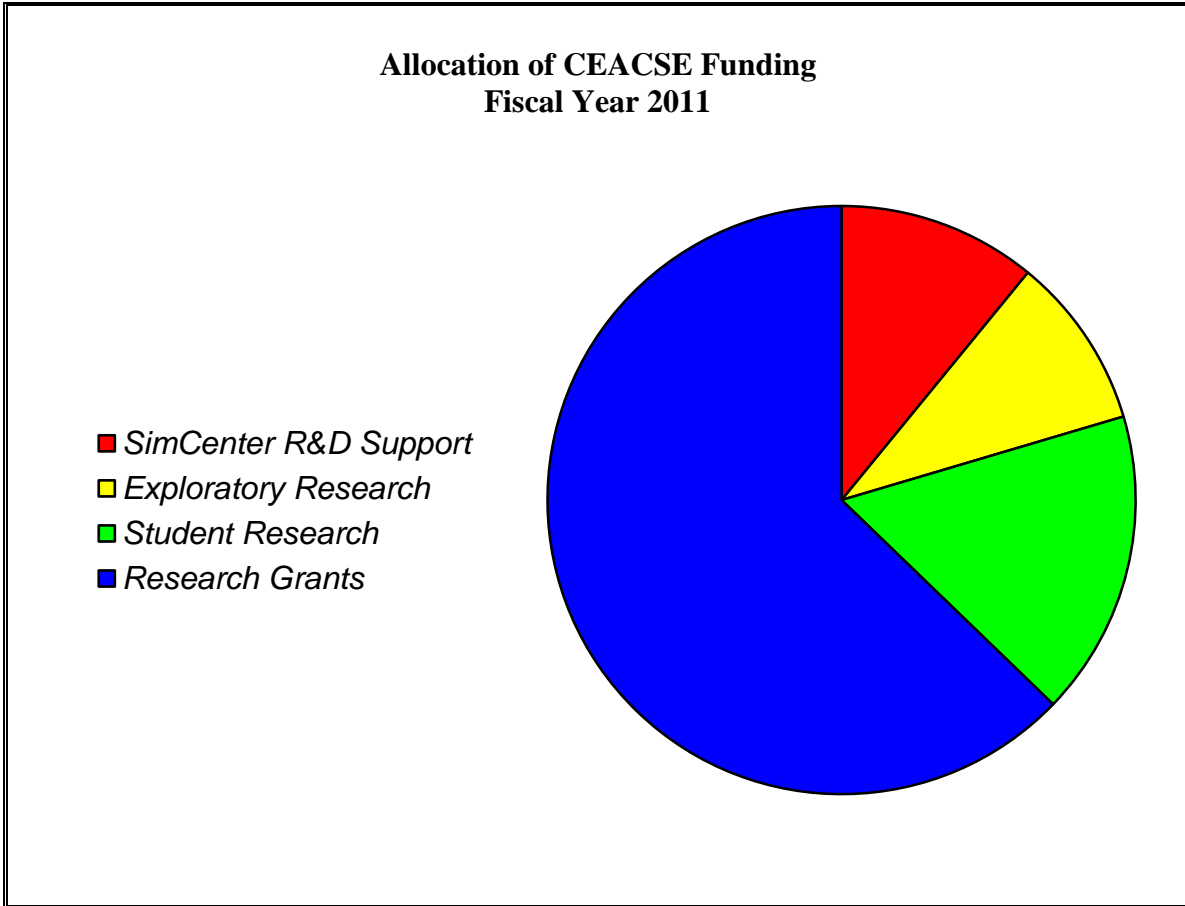
Allocation of CEACSE Funding
Fiscal Year 2011

- ■ *SimCenter R&D Support*
- ☐ *Exploratory Research*
- ■ *Student Research*
- ■ *Research Grants*

Figure 2

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

External Funding Awarded in Fiscal Year 2005-2006: $ 2,195,529

External Funding Awarded in Fiscal Year 2006-2007: $ 3,291,102

External Funding Awarded in Fiscal Year 2007-2008: $ 1,855,276

External Funding Awarded in Fiscal Year 2008-2009: $ 4,765,948

External Funding Awarded in Fiscal Year 2009-2010: $ 6,427,956

External Funding Awarded in Fiscal Year 2010-2011: $ 1,111,097

External Funding Awarded in Fiscal Year 2011-2012: $ 1,125,837

Total External Funding Awarded: **$20,772,745**

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

A multi-year view of the outcomes achieved by CEACSE is portrayed in Figure 3. The

outcome from funding provided to CEACSE by The State of Tennessee and The

University of Tennessee at Chattanooga illustrates the achievement of a two and one

half-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 FY12.

This performance has been consistent and CEACSE works toward continuous

improvement.

Multi-Year and Cumulative Research Investment Performance

State funding and external funding data shown by fiscal year: FY 05-06 ($1,132,978 and $2,195,529), FY 06-07 ($1,174,878 and $3,291,102), FY 07-08 ($1,214,378 and $1,855,276), FY 08-09 ($1,177,278 and $4,765,948), FY 09-10 ($1,298,275 and $6,427,956), FY 10-11 ($1,248,777 and $1,111,097), FY 11-12 ($1,161,648 and $1,125,837), Cummulative ($8,408,212 and $20,772,745).
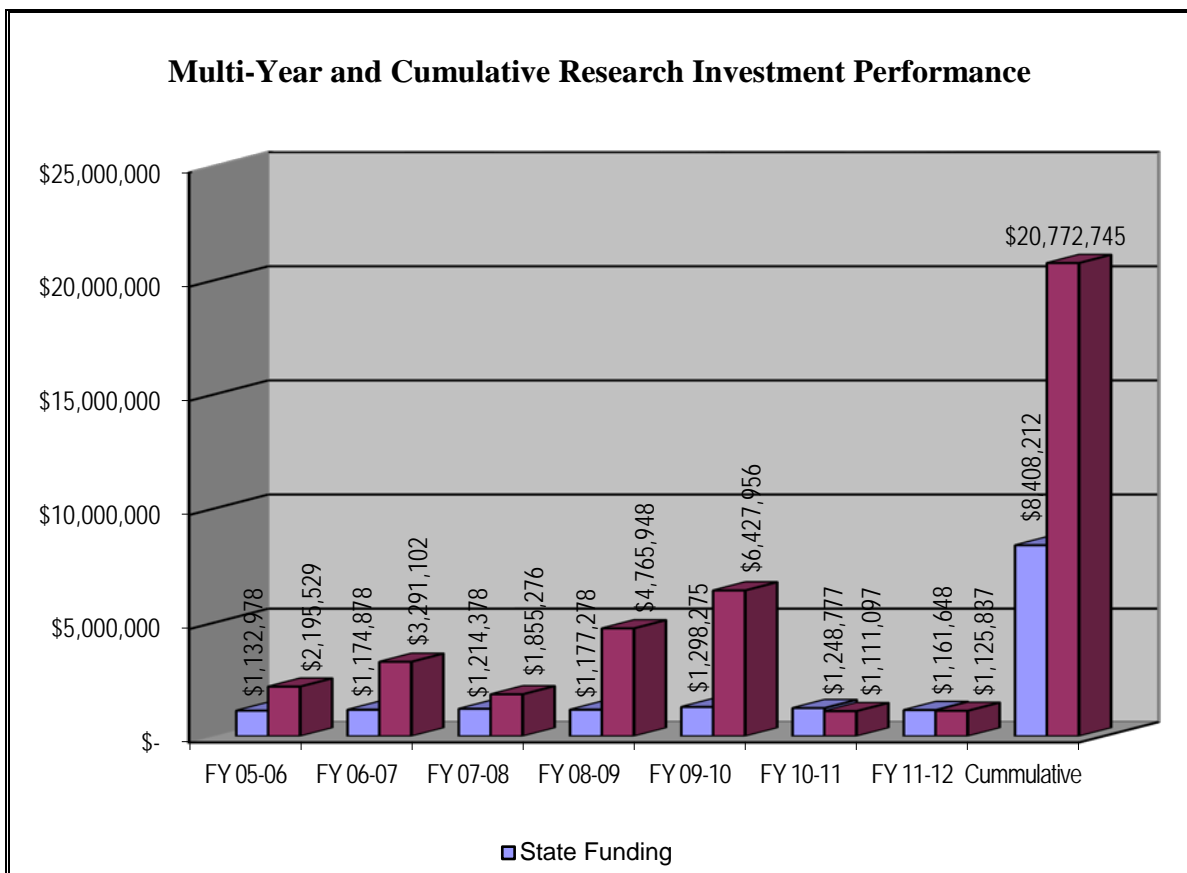
Legend: State Funding

Figure 3

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FY 2012 Publications and Presentations of the Center's Research Activities

1. Druyor Jr., C., Karman, S. "An Adaptive Hybrid Grid Generation Method for Complex Geometries", AIAA-2012-157, 50th AIAA Aerospace Sciences Meeting, Nashville, TN, January 2012.

2. O'Connell, M., Karman, S. "Techniques for Unstructured Mesh Adaptation with Elliptic Smoothing", AIAA-2012-156, 50th AIAA Aerospace Sciences Meeting, Nashville, TN, January 2012.

3. Brock, W., Burdyshaw, C., Karman, S., Betro, V., Hilbert, B., Anderson, K., Haimes, R., "Adjoint-Based Design Optimization Using CAD Parameterization Through CAPRI", AIAA-2012-968, 50th AIAA Aerospace Sciences Meeting, Nashville, TN, January 2012.

4. Mittal, A., Taylor, L.K., Sreenivas, K., and Arabshahi, A., "Investigation of Two Analytical Wake Models Using Data From Wind Farms," Proceedings of the ASME 2011 International Mechanical Engineering Congress & Exposition, Denver, Co., November 11-17, 2011.

5. Ghasemi, A., and Sreenivas, K., "On the Theory of a Novel High-Order Time-Marching Algorithm Based on Picard Iteration," UTC-CECS-SimCenter-2011-02, September 2011.

6. Anderson, W. Kyle, Wang, Li, Kapadia, Sagar, Tanis, Craig, and Hilbert, Bruce, "Petrov-Galerkin and discontinuous Galerkin methods for time-domain and frequency-domain electromagnetic simulations," J. of Comp. Physics, Vol. 230, pp. 8360-8385, 2011. DOI: 10.1016/j.jcp.2011.06.025, Available online Sept. 15, 2011.

7. Arabshahi, A., Taylor, L.K., and Whitfield, D.L. "Computation of Dynamic Stability and Control Derivatives," AIAA-2011-3348, 29th AIAA Applied Aerodynamic Conference, Honolulu, Hawaii, June 27-30, 2011.

8. Wang, L. and Anderson, W.K., "Adjoint-Based Shape Optimization for Electromagnetic Problems Using Discontinuous Galerkin Method," AIAA Journal, Vol. 49, No. 6, pp 1302-1305, 2011.

9. Wang, L. and Anderson, W.K., "Sensitivity Analysis for the Compressible Navier-Stokes Equations Using A Discontinuous Galerkin Method," AIAA-2011-3408, 41st AIAA Fluid Dynamics Conference, June, 2011, Honolulu, Hawaii.

10. Hyams, D., Sreenivas, K., Webster, R., Currier, N., "A Generalized, Unstructured Interpolative Interface method for Rotor-Stator Interactions," AIAA-2011-3700, 20th AIAA Computational Fluid Dynamics Conference, Honolulu, Hawaii, June 27-30, 2011.

11. Erwin, J. Taylor, Anderson, W. Kyle, Wang, Li, and Kapadia, Sagar, "Three Dimensional Stabilized Finite Elements for Compressible Navier-Stokes," 41st AIAA Fluid Dynamics Conference, June, 2011, Honolulu, Hawaii.

12. Nichols, III, D. S., "Accounting for Shocks in Turbulence Modeling," 41st AIAA Fluid Dynamics Conference, June, 2011, Honolulu, Hawaii.

Conclusion

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

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

Through the seed funding for research activities, undergraduate and graduate students are being engaged in a diverse range of topics. Additional efforts in this area assist in increasing the interaction and involvement of students with research faculty. Additional efforts will need to be defined, focused, and initiated to enhance/increase outreach to pre-college students. This area will receive additional and continued attention.

Finally, the role engineering and science must take in the US and Tennessee to maintain and improve our economy is increasingly apparent. CEACSE is 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.

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

Institution	UTC					Center	Center of Excellence in Applied Computional Science & Engineering		

	FY 2011-12 Actual			FY 2012-13 Proposed			FY 2013-14 Requested		
	Matching	Appropr.	Total	Matching	Appropr.	Total	Matching	Appropr.	Total
Expenditures	405,600	756,048	1,161,648	405,600	764,498	1,170,098	405,600	802,722	1,208,322
Salaries									
Faculty	246,867	458,467	705,334	246,867	458,467	705,334	239,814	465,520	705,334
Other Professional	31,813	59,082	90,895	31,813	59,082	90,895	30,904	59,991	90,895
Clerical/ Supporting	210	390	600	210	390	600	204	396	600
Assistantships	119,446	221,827	341,273	80,125	109,894	190,019	46,898	106,417	153,315
Total Salaries	398,337	739,766	1,138,102	359,015	627,833	986,848	317,820	632,324	950,144
Longevity	43	79	122	43	79	122	41	81	122
Fringe Benefits	80,107	148,770	228,877	80,108	148,771	228,879	77,818	151,059	228,877
Total Personnel	478,486	888,616	1,367,101	439,165	776,684	1,215,849	395,680	783,463	1,179,143
Non-Personnel									
Travel	3,205	5,953	9,158	3,205	5,953	9,158	3,114	6,044	9,158
Software	1,375	2,555	3,930	1,375	2,555	3,930	1,336	2,594	3,930
Books & Journals	3,891	7,227	11,118	3,891	7,227	11,118	3,780	7,338	11,118
Other Supplies			0			0			0
Equipment			0			0			0
Maintenance						0			0
Scholarships	1,741	3,232	4,973	1,741	3,232	4,973	1,691	3,282	4,973
Consultants			0			0			0
Renovation			0			0			0
Other (Specify)			0			0			0
			0			0			0
			0			0			0
			0			0			0
Total Non-Personnel	10,212	18,966	29,178	10,212	18,966	29,179	9,921	19,258	29,179
GRAND TOTAL	488,697	907,582	1,396,279	449,377	795,651	1,245,028	405,600	802,722	1,208,322
Revenue									
New State Appropriation		756,048	756,048		764,498	764,498		802,722	802,722
Carryover State Appropriation		182,687	182,687		31,153	31,153			0
New Matching Funds	405,600		405,600	405,600		405,600	405,600		405,600
Carryover from Previous Matching Funds	126,874		126,874	43,777		43,777			0
Total Revenue	532,474	938,735	1,471,209	449,377	795,651	1,245,028	405,600	802,722	1,208,322