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 2010-2011

September 26, 2011

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Executive Summary

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its sixth year of operation. The previous years have been a cornerstone in terms of 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 is fully operational. 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. There are other issues as well, several are, being the national economic environment, level of external funding committed to research and development funding and increased competitive environment. For the most part though the reporting year has proceeded smoothly with the majority of the awarded research funds being expended.

As is noted in this report, CEACSE continues to accomplish its mission and objectives. Through the awards, the researchers and associated academic units have maintained external funding from various agencies, companies, and governmental entities. CEACSE monies from the 2011 fiscal year as well as from past years continue to provide returns, reaping benefits through additional awards/grants. (Figure 1).

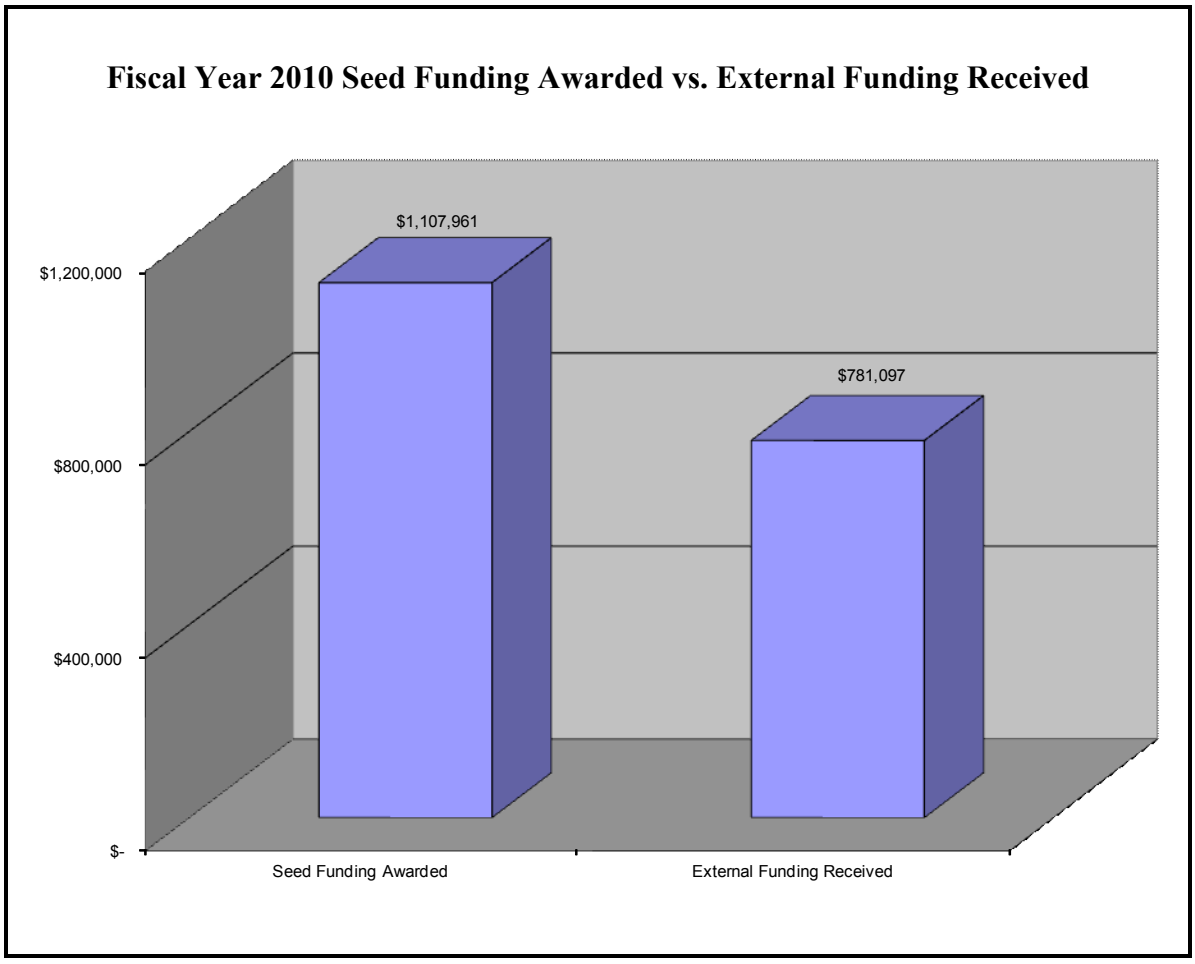

Figure 1

CEACSE continues to enhance the 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 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 2011 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 employees 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 significant augmentation of the state funding would result from federal grants and contracts in view of the expected wide interest in the resulting capability to solve problems of national interest.

Strategic Goal

The overarching goal of CEACSE is to be in accordance with the original enabling legislation and build upon the established UTC strength in applied computational science and technology to evolve into and to be recognized as a national 'Center of Excellence' and a premier multidisciplinary research and education center for computational science and engineering. CEACSE utilizes the expertise and infrastructure of the existing SimCenter staff and its computing resources. CEACSE seeds new research activities, expands previously supported research activities, and undertakes 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.

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 philosophies are continuing to achieve results (Table 1).

At the start of its sixth year, CEACSE granted funding to twenty proposed research projects. In addition, several exploratory research activities were approved and funded during Fiscal Year 2011 (Table 2). The exploratory research activities included research performed in support of requests received from external funding agencies, efforts to find external funding opportunities for a number of the CEACSE funded projects, white paper and proposal preparation assistance, and research activities undertaken by the Center's Staff. As a result of several of these opportunities being identified throughout the course of the fiscal year. One such example of exploratory research activities is small modular (nuclear) reactor (SMR)

design and development. 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 2010-2011 Research Activities

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Numerical Simulation of Lithium-Ion Batteries	$75,833	Y	$77,720	N	N	
Large Eddy Simulation of Internal Turbulent Flows	$75,434	N	$75,075	Y	N	
Implementation of the Hydrodynamic and Control System Design Technology into the Tenasi Unstructured Flow Solver	$35,549	N	$35,383	N	N	
Unstructured Elliptic Smoothing	$44,700	N	$43,330	Y	N	
Tetrahedral Mesh Creation/Optimization using Edge/Face Flips	$44,700	Y	$17,665	Y	Y	
Data Acquisition in Wireless Sensor Networks Using Distributed Rateless Codes	$40,000	N	$38.031	Y	Y	NSF CPS, $469,064 Variable Technologies LLC $15,000
Modeling turbulence Kinetic Energy for High energy Flows	$31,345	N	$28,351	Y	Y	
Targeted Mesh Adaptation for Finite Element Based Electro-Magnetics Field	$110,740	N	$94,466	Y	Y	
Spray Modeling Enhancements to the UTC Tenasi Lagrangian Particle Tracking Module	$32,573	N	$31,296	Y	N	
Profiling and Predicting Behaviors of Network-based Intrusions	$40,000	N	$37,345	Y	Y	NSF-CCLI, $99,985 NSF-SFS, $160,000 Erlanger Stroke Center, $37,048
Investigation of Boundary Conditions for Optimal Domain Size	$50,652	N	$50,625	N	N	
Investigation of Reduced Mesh Density for Resolution of Air/Water Interfaces	$70,994	N	$65,362	N	N	
Navier-Stokes Utilizing Discontinuous Galerkin/Petrov Galerkin (DG/PG) Approaches	$51,504	Y	$43,821	N	N	
Investigation of Local Low Mach Number Preconditioning Schemes	$46,127	Y	$25,801	N	N	
Physics-Based Modeling for Multi-material Interfaces	$46,127	Y	$24,637	Y	N	
Enhancing Scalability of Tenasi	$36,084	N	$35,999	N	N	
LES of Chemically Reacting Flows	$69,877	Y	$54,733	Y	N	
Direct Numerical Simulation (DNS) for a Priori Large-Eddy Simulation (LES) Sub-grid Model Evaluation	$69,877	Y	$55,310	N	N	
Propulsion Sub-System Integration Using Tenasi	$46,067	N	$30,690	Y	N	
Electromagnetic Simulations for Non-Linear Materials	$89,778	Y	$59,853	N	N	

Table 2

CEACSE Exploratory Research Activities for FY 2010-2011

Project Title	Budget	One-Year Extension	Expenses	Proposal Submitted	Externally Funded	External Funding Source(s)
Meshes for a concept Aircraft including Fan Stages		N	$4,118	N	N	
Analytical Studies of Reduced Mesh Resolution Schemes		N	$41,663	N	N	
Meteorological Model Evaluation		N	$875	N	N	
Improved Agent-Based Modeling Techniques		N	$875	N	N	
Rotorcraft Applications		N	$5,652	N	N	
Atmospheric Chemistry Modeling		N	$9,432	N	N	
Monte-Carlo Modeling		N	$8,477	N	N	
Relative Motion Meshes for Aerodynamic Simulations		N	$6,259	N	N	
Alternative Higher-Order Spatial Discretization Schemes		N	$8,594	N	N	
Low Froude Number Hydrodynamic Simulations		N	$7,532	N	N	
Atmospheric Dispersion of LNG Plumes		N	$807	N	N	
Adaptive Meshing for Aerodynamic Simulations		N	$1,750	N	N	
Turbulence Model Effects for Wind Turbine Applications		N	$1,817	N	N	
Meshes for Complete Aerodynamic Configurations		N	$3,323	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 ten Ph.D. graduate students, ten Masters level graduate students, and twelve undergraduate students. One Masters level student who worked on a grant graduated in August 2010 and is currently

pursing his Ph.D. at the University of Tennessee at Chattanooga. One Ph.D. student who graduated in May of 2011 is teaching at the University of Tennessee at Chattanooga in the College of Engineering and Computer Science. 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 six years, CEACSE faculty have made at least 393 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 TVA, Volkswagen, Babcock and Wilcox, Shaw, and Mohawk Industries. Research issues discussed included hydroelectric power generation, aerodynamic noise, heat transfer, electromagnetics, electrochemical devices, air flow management, heat element placement, drag reduction, and SMRS. 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. Research continued on improving fuel economy of large trucks by reducing aerodynamic drag. According to U.S. Xpress President Max Fuller, past work has allowed his company, one of the nation's largest trucking firms, to save 10% or $68.4M per year in fuel bills. Technical evaluation of various aftermarket trailer drag reduction devices is being performed that will assist in the down select process.

2. TVA and Babcock and Wilcox (B&W) visited the SimCenter and explained that there was growing interest in the United States in developing and using small modular reactors (SMR) in the 100 to 250 MW range instead of the larger 1500 MW type reactors currently in use. Two primary topics were discussed: 1) a simulator for the training of SMR operators at these sites, and 2) the development of a higher-fidelity simulation capability for SMRs. A proposal is being planned to address both of these issues.

3. A funding opportunity with Advanced Research Projects Agency-Energy (ARPA-E) from the Department of Energy aimed at improving our nation’s electricity transmission infrastructure was explored with TVA and Chattanooga’s Electric Power Board (EPB). The objective of this initiative is to utilize modern developments in computation, networking, and grid

monitoring to develop ways of delivering electricity more efficiently and reliably. Unfortunately the time-line for the required response of a Concept Paper was too short to be able to submit a proposal, however discussions are continuing among these groups to find a way to propose an effort to work on this urgent national problem.

Comment: An Insertion of the Establishment of SimCenter Enterprises Here?? Does it fit in this report ? Does it fit here?

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

The Center has worked to define the nature of educational outreach activities that would work to create awareness and stimulate interest in science and engineering among pre-college students. During this past year, the SimCenter conducted several events for local schools, partnering with other departments on campus and even had three high school students (1 junior, 2 seniors) intern at the SimCenter this summer preparing grids and running flow solutions on geometries of interest, including the Volkswagen Passat being manufactured here in Chattanooga. This year, the center has hosted over 700 students from Gordon Lee High School, Signal Mountain High School, Southern Adventist University, Girls, Incorporated, the Urban League STEM Academy, Independent Youth Services Foundation, GEAR UP (students from Brainerd and Howard High Schools), Chickamauga City Schools, Chattanooga School for the Arts and Sciences, Boy Scout Troop 223, Eastlake Academy, Hixson High School, All Aboard USA, and even groups of home school students. 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. 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. With partnerships that are being forged with many local schools and organizations (i.e., we have a seat on the STEM advisory board of the Urban League, the Junior Achievement Board of Directors, and the UTeaChattanooga Board of Directors and Steering Committee), more contact time, better partnerships, and thus more depth and breadth of content are on the horizon. Also, as a result of these partnerships, including one between the College of Engineering and Computer Science, the College of Health, Education, and Professional Studies, and the College of Arts and Sciences, a faculty member was awarded a grant, jointly with three others, from THEC Improving Teacher Quality funds to hold summer workshops for teachers to sharpen their knowledge of current research trends and job opportunities for their students as well as to expose them to project-based learning tools that will help capture their students' interest and give meaning to the course content.

UTC undergraduates have been recruited to work and are part of ongoing funded research projects, and this effort is continuing. Twelve undergraduates have been employed as research assistants through the most recent fiscal year. Planning efforts

continue to identify and develop additional effective outreach activities for undergraduate and graduate students, although the inclusion of an engineering course in the UHON department (UHON 1200) and a teaching presence in the undergraduate design and solid modeling classes has already gone a long way in spurring interest. Additionally, one of our faculty has been recruited to team teach a Project-Based Learning class to the UTeaChattanooga students, a group which has swelled over 100 strong in its first year, and these students are all obtaining degrees in STEM fields, including engineering, with UTC being unique in the nation in this offering.

Center Plan for Achieving Objectives

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

feasibility studies, demonstration of new capability supporting proposals, contacts with sponsoring agencies, proposal development, and related travel. This solicitation procedure is a part of CEACSE annual operating cycle.

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

Research Activities Funded by the Center

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

Extended Research Activities Funded by the Center in Fiscal Year 2009-2010 and Completed in Fiscal Year 2010-2011.

1. **Numerical Simulation of Lithium-Ion Batteries**
    - Principal 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: $75,833
    - Results: Technology development continuing and undergoing initial testing.
    -
2. **Large Eddy Simulation of Internal Turbulent Flows**
    - Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
    - Objective(s): To develop, implement, and evaluate the accuracy of models to perform large-eddy simulation of internal turbulent flows in realistic engineering configurations.
    - Seed Funding: $78,434
    - Results: Technology developed and demonstrated. Proposal submitted to NASA. Highly ranked proposal, but not selected for funding.

3. **Implementation of the Hydrodynamic and Control System Design Technology into the Tenasi Unstructured Flow Solver.**
    - Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
    - Objective(s): To implement and evaluate the hydrodynamic/aerodynamic and control system design technology into the Tenasi unstructured flow solver.
    - Seed Funding: $35,549
    - Results: Technology developed and awaiting a BAA in vehicle controls for proposal development

New Research Activities Funded by the Center in Fiscal Year 2010-2011

1. **Unstructured Elliptic Smoothing**

- Principal Investigator(s): Dr. Steve Karman, Graduate School of Computational Engineering
- Objective(s): Extend the method to control edge lengths and angles of the viscous mesh by manipulating the VCV's. Create viscous meshes by inserting boundary layer type elements into an existing mesh connectivity and use elliptic smoothing to produce the desired viscous normal distribution. Explore the manipulation of these VCV's for solution-based mesh adaptation.
- Seed Funding: $44,700
- Results: Technology developed and utilized in grid generation activities. Supporting technology for two NASA proposals and to DARPA with SRI, which were not selected for funding.

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

- Principal Investigator(s): Mr. Christopher 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. Continue the development of a surface mesh creation scheme to discretize arbitrary points typically encountered with realistic geometries. Develop interface to use tetrahedral mesher with Split-Tree based volume meshing scheme.
- Seed Funding: $44,700
- Results: Technology under development and supporting technology for NASA and DARPA with SRI proposals, which were not selected for funding.

3. Data Acquisition in Wireless Sensor Networks Using Distributed Rateless Codes

- Principal Investigator(s): Dr. Mina Sartipi, Computer Science and Engineering
- Objective(s): To provide an efficient data acquisition algorithm for WSNs, we need to solve the following problems: The transition probability matrix in random walk. The degree distribution of rateless code for compressive sensing. Recovery algorithm that works in finite/loss networks. Guessing process of our proposed recovery algorithm.
- Seed Funding: $40,000
- Results: Proposals submitted to NSF CPS and funded for $469,064. Proposal submitted to Variable Technologies LLC and funded for $15,000. Proposal submitted to NSF CAREER and NSF SHB which were not selected for funding.

4. Modeling Turbulence Kinetic Energy for High Energy Flows

- Principal Investigator(s): Dr. Stephen Nichols, Graduate School of Computational Engineering

- Objective(s): For atmospheric and hypersonic flows, turbulence kinetic energy is easily on par with the kinetic energy of the mean flow, and a proper accounting of turbulence kinetic energy in the overall energy balance is vital to accurate simulations. Shock-boundary layer interaction is an enigma that is slowly being understood, and better modeling of the Reynolds stresses in the mean flow and turbulence model computations are showing progress in recent literature in this area, and these changes will naturally enhance the simulations of highly separated flows currently being studied by the SimCenter.
- Seed Funding: $31,345
- Results: Technology developed and demonstrated. Proposal submitted to NASA. Highly ranked proposal but was not selected for funding. Proposal submitted to DARPA with SRI which was not selected for funding.

5. Targeted Mesh Adaptation for Finite Element Based Electro-Magnetics Field Solvers

- Principal Investigator(s): Dr. Chad Burdyshaw, Graduate School of Computational Engineering
- Objective(s): Develop and implement algorithms to perform error estimation and h-p mesh adaptation in an effort to improve the accuracy of scattering parameter computation for general waveguide simulation.
- Seed Funding: $110,740
- Results: Technology developed and undergoing testing.

6. Spray Modeling Enhancements to the UTC Tenasi Lagrangian Particle Tracking Module

- Principal Investigator(s): Dr. Ramesh Pankajakshan, Graduate School of Computational Engineering
- Objective(s): To enable the Lagrangian particle tracking module in the Tenasi solver to handle liquid sprays.
- Seed Funding: $32,573
- Results: Technology developed and undergoing testing. Proposal to DARPA with SRI which was not selected for funding.

7. Profiling and Predicting Behaviors of Network-based Intrusions

- Principal Investigator(s): Dr. Li Yang, Computer Science and Engineering
- Objective(s): Propose an approach to profile and predict behavior of intruders, which will enable fast detection and response against possible security breaches. Effectively detect and predict multi-step attacks. Efficiently prioritize security events based on accuracy and severity. Deliver a real application system to handle intrusions from real-world.
- Seed Funding: $40,000
- Results: Proposal submitted to NSF-SFS and funded for $160,000. Proposal submitted to NSF-MRI for $416,912 and is still pending.

Proposal submitted to NSF-SHB for $499,916 and is still pending.
Proposal submitted to NSF CCLI and funded for $99,985.
Proposal submitted to Erlanger Stroke Center and funded for $37,048.

8. Investigation of Boundary Conditions for Optimal Domain Size

- Principal Investigator(s): Dr. Abdollah Arabshahi, Graduate School of Computational Engineering
- Objective(s): To investigate and implement accurate and consistent boundary conditions for fluid dynamic or Maxwell's equations.
- Seed Funding: $50,652
  Results: Technology under development

9. Investigation of Reduced Mesh Density for Resolution of Air/Water Interfaces

- Principal Investigator(s): Dr. Dr. Robert Wilson, Graduate School of Computational Engineering
- Objective(s): Add SC artificial diffusion term to species transport and continuity equations in the Tenasi code.
- Seed Funding: $70,994
- Results: Technology developed and undergoing testing.

10. Navier-Stokes Utilizing Discontinuous Galerkin/Petrov Galerkin (DG/PG) Approaches

- Principal Investigator(s): Dr. Li Wang, Graduate School of Computational Engineering
- Objective(s): Develop and implement DG/PG methods for higher order solutions of the Navier-Stokes equations.
- Seed Funding: $51,504
- Results: Technology developed and undergoing testing.

11. Investigation of Local Low Mach Number Preconditioning Schemes

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): Explore local preconditional strategies for the compressible Navier-Stokes equations.
- Seed Funding: $46,127
- Results: Technology under development and undergoing testing.

12. Physics-Based Modeling for Multi-material Interfaces

- Principal Investigator(s): Dr. Kidambi Sreenivas, Graduate School of Computational Engineering
- Objective(s): Implement and validate multi-material interface capability in Tenasi
- Seed Funding: $46,127

- Results: Technology under development and undergoing testing. Proposal submitted to DARPA with SRI which was not selected for funding.

13. Enhancing Scalability of Tenasi

- Principal Investigator(s): Dr. Daniel Hyams, Graduate School of Computational Engineering
- Objective(s): Work collaboratively with IBM in order to get Tenasi running efficiently on a petascale-level machine.
- Seed Funding: $36,084
- Results: Technology developed and undergoing testing.

14. 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 flows. Investigate LES as applied to high-speed external flows in which dissociation reactions can become relevant. Study the injection of propane into air; though not a reacting case, this involves turbulent mixing of multiple species. Study low-speed reacting flows, an example of which is a turbulent, non premixed flame.
- Seed Funding: $69,877
- Results: Technology development continuing. Proposal submitted to DARPA with SRI was not selected for funding.

15. 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 perhaps develop new models based on the DNS results.
- Seed Funding: $69,877
  Results: Technology development continuing.

16. Propulsion Sub-System Integration Using Tenasi

- Principal Investigator(s): Dr. Robert Webster, Graduate School of Computational Engineering
- Objective(s): Use a flat plate to represent the upper surface of a blended wing body aircraft; this would all for boundary layer development and the ingestion of this boundary layer into the inlets. Investigate a single inlet-fan combination mounted on the representation of the wing-body at flight

conditions. Investigate the interaction of multiple inlets with each other and the external boundary layers.

- Seed Funding: $46,067
  Results: Technology developed and demonstrated. Proposal to NASA was a highly ranked proposal but was not selected for funding.

17. Electromagnetic Simulations for Non-linear Materials

- Principal Investigator(s): Drs. Kyle Anderson & Li Wang, Graduate School of Computational Engineering
- Objective(s): Develop higher-order accurate finite element methods for electromagnetic simulations for material properties that are dependent on the electric and magnetic fields, as well as time.
- Seed Funding: $89,778
  Results: Technology development continuing.

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 15 months.

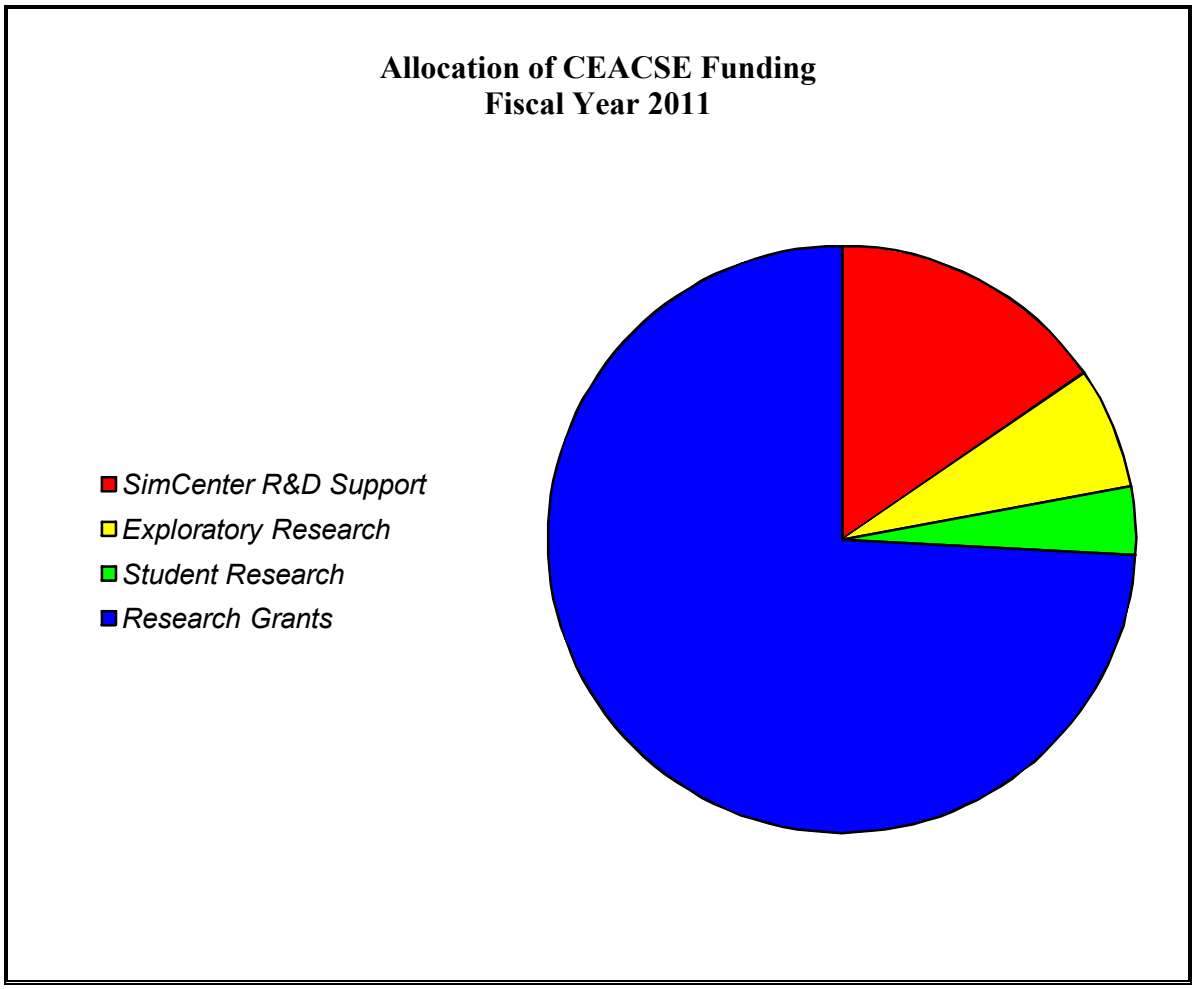

Figure 2

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

External Funding Awarded in Fiscal Year 2005-2006:	$ 2,195,529
External Funding Awarded in Fiscal Year 2006-2007:	$ 3,291,102
External Funding Awarded in Fiscal Year 2007-2008:	$ 1,855,276
External Funding Awarded in Fiscal Year 2008-2009:	$ 4,765,948
External Funding Awarded in Fiscal Year 2009-2010:	$ 6,427,956
External Funding Awarded in Fiscal Year 2010-2011:	$ 781,097
Total External Funding Awarded:	**$19,616,908**

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

A multi-year view of the outcomes achieved by CEACSE is portrayed in Figure 3. The outcome from funding provided to CEACSE by The State of Tennessee and The University of Tennessee at Chattanooga illustrates the achievement of a three-to-one ratio when compared to the amount of external funding generated by the State's investment in research. As illustrated, this rate of return continues through FY11. This performance has been consistent and CEACSE works toward continuous improvement.

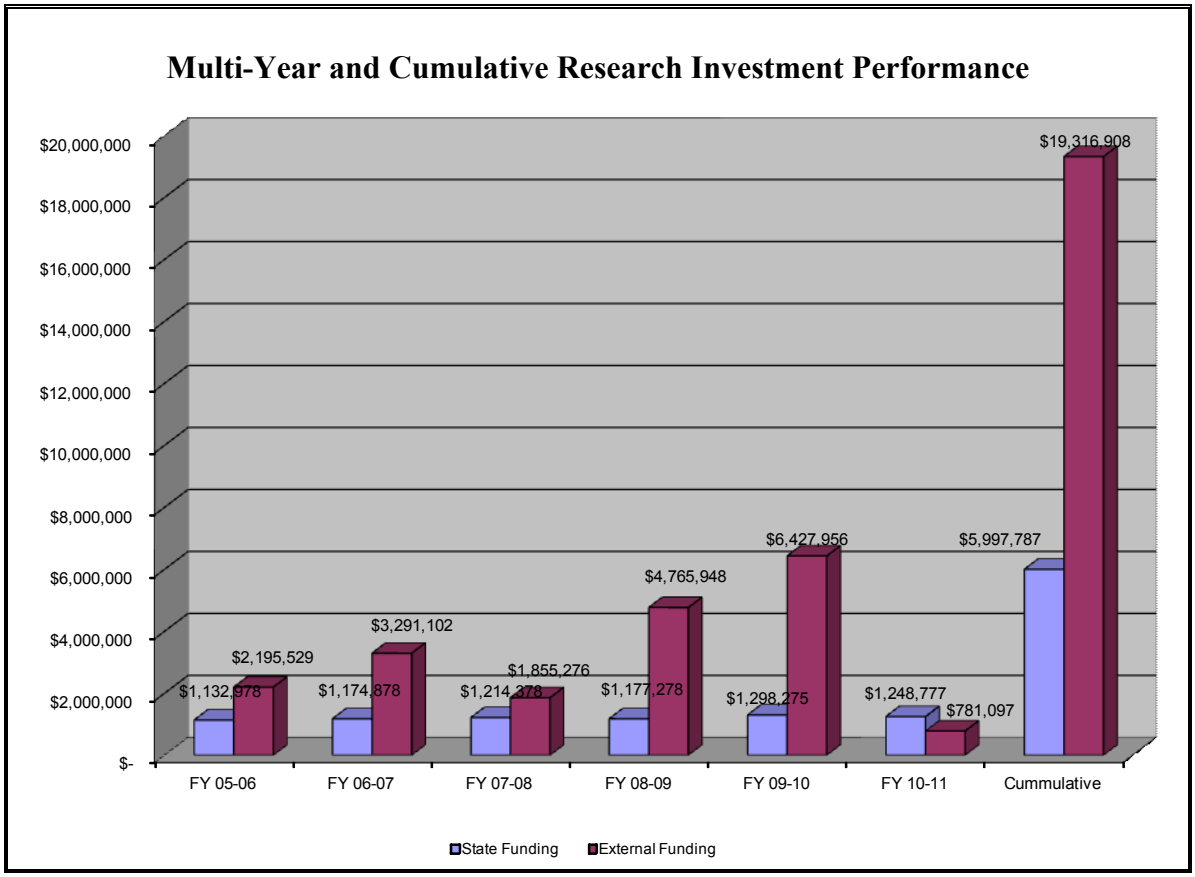

Figure 3

FY 2011 Publications and Presentations of the Center's Research Activities

- 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, Hawai, June 27-30, 2011.
- 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.
- 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.
- 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.
- Nichols, III, D. S., "Accounting for Shocks in Turbulence Modeling," 41st AIAA Fluid Dynamics Conference, June, 2011, Honolulu, Hawaii.
- Ji, L., "Unstructured Grid Technologies for Hydrodynamic Applications with Bodies in Relative Motion and Mesh Deformation," PhD Dissertation, University of Tennessee at Chattanooga, April 2011.
- Briley, W. R. and McDonald, H., "Reflections on the Evolution of Implicit Navier–Stokes Algorithms," *Computers & Fluids*, 41:15-19, 2011.
- Pankajakshan, R., Mitchell, B.J., and Taylor, L.K., "Simulation of unsteady two-phase flows using a parallel Eulerian-Lagrangian approach," *Computers & Fluids*, Volume 41, Issue 1, February 2011, Pages 20-26.
- Hyams, D.G., Sreenivas, K., Pankajakshan, R., Nichols, III, D.S., Briley, W.R., and Whitfield, D.L., "Computational simulation of model and full scale Class 8 trucks with drag reduction devices," *Computers & Fluids*, Volume 41, Issue 1, February 2011, Pages 27-40.
- Karman, Jr., S.L., "Virtual Control Volumes for Three-Dimensional Unstructured Elliptic Smoothing," AIAA-2011-893, 49th AIAA Aerospace Science Meeting, Orlando FL, January 2011.
- Betro, V. and Karman, Jr., S.L., "Fully Anisotropic Split-Tree Adaptive Refinement Mesh Generation Using Tetrahedral Mesh Stitching," *Proceedings of the 49th Annual AIAA Aerospace Sciences Meeting*, Orlando, FL, January 4-7, 2011. AIAA-2011-0895.
- Kapadia, S., Anderson, W.K., and Burdyshaw, C., "Channel shape optimization of solid oxide fuel cells using advanced numerical techniques," *Computers & Fluids*, Vol. 41, 2011, 41-50.Masters, J. S., "Winslow Elliptic Smoothing Equations Extended to Apply to General Regions of an Unstructured Mesh," PhD Dissertation, University of Tennessee at Chattanooga, December 2010.
- Wang, L., Mavriplis, D.J., and Anderson, W.K., "Adjoint Sensitivity Formulation for Discontinuous Galerkin Discretizations in Unsteady Inviscid Flow Problems," *AIAA Journal*, Vol. 48 (12), 2010.
- Betro, V., "Implementing a Node-Based Split-Tree Neighbor Search Algorithm," Research Note, 19th Annual International Meshing Roundtable, Chattanooga, TN, October 6-8, 2010.

- Karman, S.L. Jr., "Virtual Control Volumes for Two-Dimensional Unstructured Elliptic Smoothing," 19th International Meshing Roundtable, paper 2A.4, Chattanooga, TN, October, 2010.
- Hyams, Daniel G., Kress, Reid, and Swafford, Tim W., "CFD-Driven Agent-Based Dispersion Modeling of the Y-12 National Security Complex," UTC-CECS-SimCenter-2010-01-R, September 2010.
- Ji, L., Sreenivas, K., Hyams, D., and Wilson, R., "A Parallel Universal Mesh Deformation Scheme for Hydrodynamic Applications," *Proceedings of the 28th ONR Symposium on Naval Hydrodynamics*, Pasadena, CA, 12-17 Sep. 2010.
- Betro, V. C., "Fully Anisotropic Split-Tree Adaptive Refinement Mesh Generation Using Tetrahedral Mesh Stitching," PhD Dissertation, University of Tennessee at Chattanooga, August 2010.

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 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 needs additional and continued attention.

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

Schedule 7

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

Institution UTC **Center** **App. Computional Science & Eng**

	FY 2010-11 Actual			FY 2011-12 Proposed			FY 2012-13 Requested		
	Matching	**Appropr.**	**Total**	**Matching**	**Appropr.**	**Total**	**Matching**	**Appropr.**	**Total**
Expenditures	405,600	843,177	**1,248,777**	405,600	756,482	**1,162,082**	405,600	794,306	**1,199,906**
Salaries									
Faculty	255,035	541,949	**796,985**	305,799	543,644	**849,443**	280,500	544,500	**825,000**
Other Professional	18,496	39,305	**57,801**	23,400	41,600	**65,000**	18,700	36,300	**55,000**
Clerical/ Supporting			**0**	3,600	6,400	**10,000**			**0**
Assistantships	31,400	66,726	**98,126**	72,000	128,000	**200,000**	10,200	19,800	**30,000**
Total Salaries	**304,932**	**647,980**	**952,911**	**404,799**	**719,644**	**1,124,443**	**309,400**	**600,600**	**910,000**
Longevity	37	79	**115**	72	128	**200**	102	198	**300**
Fringe Benefits	73,542	156,277	**229,819**	100,800	179,200	**280,000**	84,866	164,740	**249,606**
Total Personnel	**378,511**	**804,335**	**1,182,846**	**505,671**	**898,972**	**1,404,643**	**394,368**	**765,538**	**1,159,906**
Non-Personnel									
Travel	1,717	3,650	**5,367**	5,400	9,600	**15,000**	5,100	9,900	**15,000**
Software	32	68	**100**	3,600	6,400	**10,000**	3,400	6,600	**10,000**
Books & Journals			**0**	1,080	1,920	**3,000**	340	660	**1,000**
Other Supplies	837	1,778	**2,614**	1,800	3,200	**5,000**	680	1,320	**2,000**
Equipment			**0**			**0**			**0**
Maintenance			**0**			**0**			**0**
Scholarships	1,535	3,261	**4,796**	7,200	12,800	**20,000**	1,032	8,968	**10,000**
Consultants			**0**	3,600	6,400	**10,000**			**0**
Renovation			**0**			**0**			**0**
Other (Specify)			**0**			**0**			**0**
Printing	249	529	**778**	360	640	**1,000**	170	330	**500**
Communications	789	1,676	**2,465**	1,080	1,920	**3,000**	510	990	**1,500**
			0			**0**			**0**
Total Non-Personnel	**5,158**	**10,962**	**16,120**	**24,120**	**42,880**	**67,000**	**11,232**	**28,768**	**40,000**
GRAND TOTAL	**383,669**	**815,297**	**1,198,966**	**529,791**	**941,852**	**1,471,643**	**405,600**	**794,306**	**1,199,906**
Revenue									
New State Appropriation		843,177	**843,177**		756,482	**756,482**		794,306	**794,306**
Carryover State Appropriation		154,807	**154,807**		182,687	**182,687**			**0**
New Matching Funds	405,600		**405,600**	405,600		**405,600**	405,600		**405,600**
Carryover from Previous Matching Funds	104,943		**104,943**	126,874		**126,874**			**0**