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 2006-2007

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## Executive Summary

The Center of Excellence in Applied Computational Science and Engineering (CEACSE) has recently completed its second year of operation. These first two years have been the cornerstone in terms of the establishment and development of an effective operation. This also has been a period of inculcating a culture of the securing external funding as an outcome of seed research funding provided by CEACSE. There have been some initial challenges as the Center became operational. One primary challenge was the necessity to provide one-year extensions to researchers who were awarded seed funding in the first year of CEACSE. Year two, for which this report is filed, has proceeded smoothly with previous first-year funding as well as second-year funding being expended appropriately during this report period.

As is noted in this report, CEACSE is accomplishing its mission and objectives. Through the awards issued, the researchers and their units have received funding from various agencies, companies, and governmental entities. The total of the awards has approached a two-to-one return on the monies provided to CEASE. Approximately 93% of the external funding awarded to researchers has resulted from the seed funding provided by CEACSE to the researcher.

CEACSE continues to seek to enhance the education aspect of students through the Ph.D. and M.S. graduate programs at the University of Tennessee at Chattanooga. Both graduate and undergraduate students have been utilized on various research activities

undertaken as a result of CEACSE funding. The SimCenter at Chattanooga continues to be an anchor and attract students locally as well as nationally and internationally.

Finally as a result of funding research activities and secured external funding, several companies have chosen to locate an office here in the Chattanooga area. This component of CEACSE's objectives is a continuing effort. As CEACSE's activities and accomplishment become more widely known, this component will gain additional traction in development and growth.

Finally, a current review of CEACSE and Advisory Board comments is presented in the section entitled, "Program Review Board Report". This section encompasses the Advisory Board's recent review, including CEACSE's briefing charts, and a short biography of each board member.

The following is the Annual Report FY 07 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 a timely opportunity to capitalize on the successful initiative of the UT Computational Simulation and Design Center at Chattanooga (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 UT SimCenter at Chattanooga and the Graduate School of Computational Engineering. The CEACSE builds upon this expertise to broaden and deepen the concept of a computational simulation center to consider a wider array of practical problem areas in science and engineering. This enlargement has involved additional faculty from across the University, particularly in areas of science and engineering, and has been based on the use of advanced computational methodologies to solve complex practical problems in applied science and engineering. The particular applications selected are of interest to local industries and state and federal agencies. While funding for the Center seeds these activities, it anticipates that significant augmentation of the state funding would result from federal grants and contracts in view of the expected wide interest in the resulting capability to solve problems of national interest.

## CEACSE Description

### *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 become recognized as a national 'Center of Excellence' and a premier multidisciplinary research and education center for computational science and engineering. CEACSE utilizes the expertise and infrastructure of the existing SimCenter staff and its computing resources. CEACSE seeds new research activities, expands previously supported research activities, and undertakes activities that lead to additional sources of funding. Appropriate faculty across the entire University and particularly those in science and engineering are involved. Thus the research portfolio broadens research contributions made that 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 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 UT SimCenter at Chattanooga with its expertise in computational science and applications methodologies that are broadly applicable both in new problem areas and in other 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*

1. *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 made operational a significant cluster super computer. This machine has been configured to perform and support computational simulations on large complex problems. It is also has a significant rating when compared to other such supercomputers nationally and worldwide (Figure 1).

**UT SimCenter Ranking Among TOP500 Supercomputer Sites Worldwide***

Cluster has 1,010 3.2 GHz Intel processors, 1.01 Terabytes Memory, and 20.8 Terabytes Disk Space and places UTC

- 457th in the World
- 256th in the U.S.

*Based on June 2007 TOP500 Supercomputer Site Rankings

**Figure 1**

To this end there has been a large expansion of capabilities to broaden research and support activities. During its first year, CEACSE enabled the expansion of research explorations and activities across the University faculty and SimCenter researchers through its seed funding to achieve subsequent external funding. 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 research or related research. Through the first year operation it could be seen that the Center's funded activities and philosophy were beginning to achieve results (Table 1).

At the start of its second year, CEACSE granted one-year no cost extensions to the previous year's funded research activities. Due to delays in the initial proposals and awards process, many of the funded research activities were not able to begin their research until the middle of that fiscal year. The extensions were granted in order to give the principal investigators ample time to meet their research goals and apply for external funding.

In addition to the research activities carried over from the previous fiscal year, a new project was granted seed funding and several exploratory research activities were approved and funded during FY06-FY07 (Table 2). The exploratory research activities included research performed in support of requests received from external funding agencies, efforts to find external funding opportunities for a number of the CEACSE funded projects, white paper and proposal preparation assistance, research activities undertaken by the Center's Staff, and several of these opportunities were

identified during the course of the fiscal year (outside the normal cycle). These did not go through the normal proposal process and were initiated at the discretion of the Center's Director. The Center has also provided funding for graduate and undergraduate student research.

**Table 1**

***CEACSE Seed Funding Committed for FY 2005-2006 Research Activities***

| Project Title | Budget | One-Year Extension | Expenses | Proposal Submitted | Externally Funded | External Funding Source(s) |
|---|---|---|---|---|---|---|
| Quantum Measurement and Feedback in Atomic Systems | $ 18,420 | Y | $ 16,399 | Y | N | |
| Information Communication Mediator Model in Disaster Management | $ 33,250 | Y | $ 29,190 | Y | N | |
| A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysts | $ 37,870 | Y | $ 36,833 | Y | N | |
| Geometry Manipulation and Visualization, Computational Simulation and Design | $ 59,109 | Y | $ 62,683 | Y | Y | NASA Langley, NASA Glenn |
| Unstructured Solution Algorithm System Integration, Design and Testing | $ 66,550 | Y | $ 62,696 | Y | Y | Dept. of Energy, Office of Naval Research, Aerospace Testing Alliance, NASA Glenn |
| Multiprocessor Objective-C computer Systems for High Performance Computing | $ 61,200 | Y | $ 45,382 | | N | |
| Numerical Solution of the Boltzmann Equation with BGK Approximation | $ 74,600 | N | $ 73,285 | Y | N | |
| Adjoint Method for Magnetohydrodynamic Simulations | $ 95,391 | Y | $ 94,778 | Y | Y | Coronal Energy |
| Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers | $ 96,255 | Y | $ 96,225 | Y | Y | Office of Naval Research, Riverbend Technology Institute, Jackson & Tull/Air Force Research Lab |
| Development of an Unstructured Grid Algorithm for Turbomachinery† | $ 98,318 | Y | $105,633† | Y | Y | Office of Naval Research, Aerotonomy, NASA Glenn |
| Advancement and Verification of the Navier-Stokes Flow Solver for Rocket Motor† | $100,078 | Y | $107,175† | Y | Y | Science & Technology Applications, Jackson & Tull/Air Force Research Lab |
| Computational Engineering with Solid Oxide Fuel Cells* | $110,000 | Y | $153,700* | Y | Y | The Enterprise Center/Small Business Administration |
| Evaluation and Enhancement of an Unstructured Grid Algorithm for Free Surface† | $116,160 | Y | $100,260† | Y | Y | Office of Naval Research |
| Computational Analysis and Design of Fuel Cell Components | $124,329 | Y | $123,501 | Y | Y | The Enterprise Center/Small Business Admin. |
| Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing | $148,298 | Y | $148,145 | Y | Y | Office of Naval Research, Science & Technology Applications, NASA Langley, NASA Glenn |
| Advanced Turbulence Modeling for Unstructured Topologies | $166,056 | Y | $164,415 | Y | Y | Department of Energy, Office of Naval Research |
| Computation of Dynamic Stability and Control Devices | $168,250 | Y | $162,241 | N | N | |
| Computational Methods for Field Simulations | $168,445 | Y | $168,881 | Y | Y | Coronal Energy, Aerospace Testing Alliance, Aerotonomy, NASA Glenn, Radiance Tech. |

Table 1 Notes:

† Upon receipt of external funding, the research grant entitled "Evaluation and Enhancement of an Unstructured Grid Algorithm for Free Surface" had a budget surplus. At the request of the Department Head of the Principal Investigators, the budget surplus was split between two research grants facing budget shortfalls in order to allow those projects to continue and seek external funding. Proposals from both of those research grants were subsequently awarded external funding.

* Receipt of the external funding awarded for work performed on this research grant was delayed by the funding agency. The budget for this research project was increased in the interim in order to allow the Principal Investigator to continue his research and to allow the student researchers to complete their research topics.

**Table 2**

***CEACSE Research Activities for FY 2006-2007***

| **Seed Funding** | **Budget** | **One-Year No-Cost Extension** | **Expenses** | **Proposal Submitted** | **Externally Funded** | **External Funding Source(s)** |
|---|---|---|---|---|---|---|
| Kinetic Simulation of Multispecies Gas Flows on Unstructured Grids | $ 85,500 | N | $ 80,082 | | | |
| **Exploratory Research Activities** | | | | | | |
| Validate Equilibrium Chemistry Capability | | | $ 27,978 | Y | Y | Science & Technology Applications, Jackson & Tull/Air Force Research Lab |
| Implement Sensitivity Analysis Capability for Validated Equilibrium Chemistry Model | | | | | | |
| Implement Sensitivity Analysis Capability | | | | | | |
| Apply Newly Developed Capabilities to a Converging-Diverging Nozzle Geometry | | | | | | |
| Perform Grid Sensitivity Study/Grid Resolution Study for Converging/Diverging Nozzle Geometry | | | | | | |
| Fuel Cell Demonstration Project | | | $ 78,461 | Y | Y | The Enterprise Center/Small Business Admin. |
| Assistance in identifying external funding opportunities and proposal preparation | | | $ 81,649 | | | |

In order to ensure that the objectives of the Center's investment are being 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

2. *A secondary objective is to increase the participation of additional faculty, graduate and undergraduate students in the Center's research efforts and where possible assist in the recruitment of new faculty and students to the University.*

CEACSE has continued the success seen in its first year in being able to broaden the scope of research through increased participation of additional faculty, graduate students and undergraduate students.

CEACSE continued seed funding for 17 faculty members from various disciplines, such as physics, computer science, and computational engineering, who were involved in seed research funding activities. New seed funding was provided for one Ph.D. level student who is also a staff member. Many of these projects have led to significant external funding awards.

CEACSE funding has continued the support of seven Ph.D graduate students, thirteen Masters students, and eight undergraduate students. One Ph.D. student working under a seed grant graduated in August 2007 and has accepted a postdoctorate position at the University. One Masters student who worked on a seed grant graduated in December 2006 and is currently pursing his Ph.D. at the University of California, Santa Barbara. Two Masters students supported by seed funding have graduated and will continue their studies towards a Ph.D. at the University of Tennessee at Chattanooga. Another Masters student supported by two seed funding research grants, and who started as an Undergraduate student working on these grants, has recently accepted a research staff position with the University of Tennessee at Chattanooga. One undergraduate research assistant received a national research award for work that she performed on a CEACSE research grant. This same student has decided to pursue her Masters degree in Bioengineering at The Johns Hopkins University.

3. *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 many companies visit and discuss opportunities for collaboration on research. Additionally, the Center been involved in many meetings hosted at the UT SimCenter at Chattanooga, on the UTC campus. Another example of results from

this objective are that two companies (Radiance Technologies, Inc. and Adaptive Methods) have opened offices in Chattanooga since research activities are available. Additionally through research activities supported by CEACSE, opportunities are created for the education of graduate students, thereby providing the students the potential to secure high paying and quality positions and to be able to remain within Tennessee.

4. *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.*

In this first year of operation, the Center worked to define the nature of educational outreach activities that would work to create awareness and stimulate interest among pre-college students. One Chattanooga area high school has had students visit and interact with the researchers at the UT SimCenter. The SimCenter has hosted visits for two groups of about twenty high-school students from Girls, Inc. for the purpose of promoting awareness and stimulating interest in the study of mathematics, science, and engineering.

Additional types of outreach continue to be investigated. These activities to elementary, middle and high schools continue to be softer than desired. UTC undergraduates have been recruited to work and are part of ongoing funded research

projects, and this effort is continuing. Five undergraduates have been employed as research assistants through the first year. One of these undergraduates is now a M.S. student in the UTC Computational Engineering program. Planning efforts continue to identify and develop additional effective outreach activities for undergraduate and graduate students.

***Center Plan for Achieving Objectives***

The operation of the Center is guided by strategic planning to identify promising research avenues within the broad area of applied computational science and engineering. Some promising areas have been identified that leverage existing research capabilities into new and related areas. The Center continues to seek ongoing participation from other UTC faculty and personnel to identify additional areas of strength based on their individual expertise and synergism with other Center activities. The Center has solicited 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) increased in national and international stature, and d) promoted 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.

*New Research Activities Funded by the Center in Fiscal Year 2006-2007*

**1. Kinetic Simulation of Multispecies Gas Flows on Unstructured Grids**

- PI: Mr. R. Glenn Brook, UT SimCenter at Chattanooga, Ph.D. student
- To develop a parallel, implicit, unstructured, finite-volume flow solver for the Boltzmann-BGK equation that supports multispecies fluid flows to enable future research into chemically reactive nanoscale flows.
- Results: Notification to CEACSE is pending regarding any proposals and external funding. Final report is due for submission.

Total Seed Funding: $85,500

*Extended Research Activities Funded by the Center in Fiscal Year 2005-2006 and Completed in Fiscal Year 2006-2007*

**1. Information Communication Mediator Model in Disaster Management**

- PI: Dr. Li Yang and Dr. Joseph Kizza, College of Engineering and Computer Science
- Provide timely, secure and dependable communication between public health and safety agencies in the face of the natural disaster or man-made disaster; and provide a methodology to specify, analyze and validate the prototypes in real-time distributed data access and assistive computer technology.
- Results: Dr. Yang and Dr. Kizza submitted proposals for external funding to the Defense Threat Reduction Agency, Oak Ridge National Laboratory, and two to the National Science Foundation. None of the proposals were funded. They are currently teaming with seven other universities to submit NSF CI-TEAM proposal. The results of this proposal will not be available until next year.

**2. Multiprocessor Objective-C computer Systems for High Performance Computing**

- PI: Dr. Andrew Novobilski, College of Engineering and Computer Science
- Support the development of a Multiprocessing Objective-C Compiler System (MOCS) that includes native language support for distributed, event-based, scientific computing applications. This tool will be a first implementation of a necessary component, the ability to transparently apply High Performance Computing to large data set problems, in the current research being carried out by the Principal Investigator in conjunction with several emergency room physicians.

- Results: Research activities undertaken early in research initiation stage currently have been suspended due to the principal investigator being on a one-year assignment at another university. No proposal or final report has been submitted. No external funding has been received.

**3. Computational Methods for Field Simulations**

- PI: Dr. W. Roger Briley, Graduate School of Computational Engineering
- Identify new applications whose underlying physical processes have mathematical models that are sufficiently well developed to justify large-scale computational simulations, both as a tool for improving physical understanding and for efficient and effective low-cost problem solutions. Possible areas of new research include alternative energy sources, nanotechnology, biotechnology, electromagnetics, atmospheric and ocean sciences, and hydrology. New areas of research that are linked to local companies or regional economic development will be a high priority. Possible opportunities exist with Black Light Power, Radiance Technologies, Adaptive Methods, and Aerotonomy, Inc.
- Results: Dr. Briley's work contributed to the submission of the following proposals which were funded for total of $2,242,000.
    - A proposal to the NASA NRA program which was selected for an award of $1,500,000 over three years, beginning in Fall 2007.
    - A proposal to support Aerotonomy's Air Force SBIR Phase II proposal. The proposal was awarded $75,000.
    - A proposal to Radiance Technologies, Inc. which was awarded $450,000.

- A proposal to Coronal Energy, LLC which was funded for up to $192,000.
- A proposal to Aerospace Testing Alliance which was funded for $25,000.

**4. Advanced Turbulence Modeling for Unstructured Topologies**

- PI: Dr. D. Stephen Nichols III, UT SimCenter at Chattanooga
- Develop a high-fidelity computational capability for numerically simulating highly separated, turbulent fluid flows that are frequently encountered in real world problems. This research will advance the capabilities of the SimCenter in computational simulation and design of fluid-dynamic phenomena involving highly separated, turbulent fluid flows about complex configurations. In particular, the study of urban environmental flows, of global and regional climate modeling, of atmospheric transport and diffusion of pollutants, and of large vehicle drag reduction will be greatly enhanced. Consequently the University's potential will be enhanced by improving its marketability to industry and government agencies such as DOE, DOD, and Homeland Security.
- Results: Dr. Nichols' work contributed to the submission of the following proposals which were funded for total of $1,635,000.
  - A proposal to the Department of Energy which was awarded $579,000.
  - A proposal to the Office of Naval Research which was awarded $1,056,000.

**5. Unstructured Solution Algorithm System Integration, Design and Testing**

- PI: Dr. Daniel Hyams, Graduate School of Computational Engineering
- Provide a consistently stable software platform in order to effectively offer the technological capabilities of the SimCenter to potential sponsors. Produce an integrated software implementation of all unstructured technologies that can be used in conjunction with all proposed projects. In addition, a full suite of verification results as well as an automated testing engine are to be implemented, such that any anomalous behavior of the software implementation is isolated within a short time frame.
- Results: Dr. Hyams' work contributed to the submission of the following proposals which were funded for total of $3,160,000.
    - A proposal to the Department of Energy which was awarded $579,000.
    - A proposal to the Office of Naval Research which was awarded $1,056,000.
    - A proposal to Aerospace Testing Alliance which was funded for $25,000.
    - A proposal to the NASA NRA program which was funded for $1,500,000.

**6. Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers**

- PI: Dr. Ramesh Pankajakshan, UT SimCenter at Chattanooga
- Develop a high-fidelity computational capability for numerically simulating the fluid mechanics of two phase flow consisting of particulate matter being transported by the gas phase. The two-phase flow module would expand the capabilities of flow codes to problems ranging from pollutant transport to rocket engines. The new capabilities

would be of interest to government agencies such as DOD,DOE, EPA and DHS as well as the process and aerospace industries.

- Results: Dr. Pankajakshan received $100,000 funding from the Riverbend Technology Institute to apply his research to problems regarding the aerodynamics of ground vehicles. Dr. Pankajakshan's work also contributed to the submission of proposals to the Office of Naval Research which was awarded $1,056,000 and to Jackson & Tull/Air Force Research Laboratory which was awarded $180,000.

**7. Quantum Measurement and Feedback in Atomic Systems**

- PI: Dr. Jin Wang, Department of Physics, Geology & Astronomy
- Develop a theoretical and computational framework for the design and analysis of quantum feedback control systems. To study the steady-state entanglement in a two qubit system using quantum measurement and feedback in order to find an analytical solution for the steady-state entanglement using a homodyne-mediated feedback scheme.
- Results: Dr. Wang submitted a proposal for external funding to the National Science Foundation in September 2006 and a proposal to the Research Corporation in November 2006. Neither of these proposals was funded.

**8. Evaluation and Enhancement of an Unstructured Grid Algorithm for Free Surface**

- PI: Dr. Robert Wilson, UT SimCenter at Chattanooga
- Test and further develop an unstructured flow solver for simulation of turbulent free surface flow over complex geometries, including military and commercial ships. The computational tool will be used to investigate high speed flow over ships with breaking waves. This research will advance the capabilities of the computational simulation of free surface flows and ship design. When combined with hull form optimization techniques, the approach could be used to reduce ship resistance, free surface signatures, and propeller performance. This research which will greatly enhance the potential and marketability of the computational tool to industry and government agencies such as the DOD, DOE, and Homeland Security in general, and in particular, the Office of Naval Research. Furthermore, this project will involve and educate students in basic free surface modeling and hydrodynamic, as well as dynamic ship response to environmental conditions.
- Results: Dr. Wilson's work contributed to the submission of a proposal to the Office of Naval Research which was awarded $1,056,000.

**9. Computation of Dynamic Stability and Control Devices**

- PI: Dr. Abdollah Arabshahi, UT SimCenter at Chattanooga
- Develop a predictive technology to support virtual design and evaluation of underwater vehicles systems, employing a Computational Fluid Dynamics (CFD) based methodology for predicting stability and control derivatives. Computational Fluid Dynamics technology coupled with modeling and control system design will allow vehicle conceptual designs to be evaluated within the context of a realistic mission. The preliminary goal of this effort is to estimate stability and control derivatives of underwater vehicles from CFD data as an evaluation of the potential for this method to replace/reduce expensive experimental (i.e. tow-tank) tests. The results of the study will be used to improve the performance of underwater vehicles.
- Results: A final report has been submitted for this research activity. Notification of results from any proposal(s) is pending.

**10. A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysts**

- PI: Dr. Frank Jones, College of Engineering and Computer Science
- Perform computer simulations to study the fundamental effects of changing the size, shape, location, and density of packing particles on conversion in microchannels in order to develop the ability to design a packing structure for optimum conversion. This ability should be of great economic value to the micro and non device community.

- Results: Dr. Jones submitted a proposal for external funding to the Petroleum Research Fund (an American Chemical Society agency). This proposal was not funded. Dr. Jones is currently preparing a proposal for submission to the National Science Foundation. The results of this proposal will not be available until next year.

**11. Geometry Manipulation and Visualization, Computational Simulation and Design**

- Co-PIs: Ms. Dawn Ellis, College of Engineering and Computer Science and Dr. Steve Karman, Graduate School of Computational Engineering
- Develop a platform independent console to facilitate the computational design process. Specific objectives include the ability to input geometry from a CAD package to prepare for meshing; the ability to define boundary constraints, group boundaries and define design variables based on the CAD model; the ability to place constraints to ensure geometric usability, and the ability to manage the overall design process by monitoring cost, gradients and constraints.
- Results: Ms. Ellis and Dr. Karman submitted a proposal for external funding to NASA Langley Research Center. The proposal was awarded a three-year contract for $700,674. Dr. Karman and Ms. Ellis' work also contributed to a proposal submitted to NASA Glenn Research Center which was awarded $1,527,072 over three years.

**12. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing**

- PI: Dr. W. Kyle Anderson and Dr. Steve Karman, Graduate School of Computational Engineering
- Develop an adjoint solver based on the existing unstructured mesh solver in the SimCenter which will be discretely consistent with the flow solver and which will be "self maintaining" in that changes in the analysis code will be automatically reflected in the adjoint solver. Once developed, the adjoint solver will be used for sensitivity analysis, design, error estimation, and adaptive meshing.
- Results: Dr. Anderson and Dr. Karman's work contributed to the following proposals for external funding which were funded for total of $3,765,631.
    - A proposal submitted to the The Enterprise Center and Small Business Administration which was awarded a contract for $456,529.
    - A proposal submitted to the Office of Naval Research which was awarded $1,056,000.
    - A proposal submitted to NASA Langley Research Center which was awarded a three-year contract for $700,674.
    - A proposal submitted to NASA Glenn Research Center which was awarded $1,527,072 over three years.
    - A proposal submitted to Science & Technology Applications which was awarded $25,356.

**13. Adjoint Method for Magnetohydrodynamic Simulations**

- PI: Dr. W. Kyle Anderson and Dr. Steve Karman, Graduate School of Computational Engineering
- Develop computational methods for numerically simulating problems involving magnetohydrodynamics. This capability would provide the ability to simulate MHD problems where the results have quantitatively known levels of accuracy. The results can be used to support research in fusion.
- Results: Dr. Anderson and Dr. Karman's work contributed to a proposal for external funding submitted to Coronal Energy, LLC. The proposal was funded up to $192,000.

**14. Computational Analysis and Design of Fuel Cell Components**

- PI: Dr. W. Kyle Anderson and Dr. Steve Karman, Graduate School of Computational Engineering
- Use numerical simulations to analyze and improve fuel cell components that are considered critical for advancing the technology to the point where fuel cells become a viable means of producing power for industrial applications.
- Results: Dr. Anderson and Dr. Karman's work contributed to a proposal for external funding submitted to The Enterprise Center and Small Business Administration which was awarded a contract for $456,529.

**15. Computational Engineering with Solid Oxide Fuel Cells**

- PI: Dr. James Henry, College of Engineering and Computer Science
- Enable a thorough investigation and analysis of the modeling, operation and performance of the Solid Oxide Fuel Cell (SOFC) used in the Chattanooga Fuel Cell Demonstration project funded by the Department of Energy. The computer engineering and technical infrastructure is vital to the success of the Chattanooga Fuel Cell Demonstration project. The equipment control, data acquisition and communication of performance are all totally dependent upon reliable and effective computer hardware and software.
- Results: Dr. Henry's work contributed to a proposal for external funding submitted to The Enterprise Center and Small Business Administration which was awarded a contract for $456,529.

**16. Advancement and Verification of the Navier-Stokes Flow Solver for Rocket Motor Internal Flows**

- PI: Dr. Abdollah Arabshahi, UT SimCenter at Chattanooga
- Provide a computational analysis tool in support and development of modeling and simulation of solid propellant rocket motors (SRMs) by government agencies and industry. To assess the current capability of the flow solver when applied to a basic internal flow problem with wall blowing and to enhance the capability of the solver to simulate flow representative of the internal flow of SRMs.

- Results: Dr. Arabshahi's work contributed to the following proposals for external funding which were funded for total of $205,356.
    - A proposal submitted to Science & Technology Applications which was awarded $25,356.
    - A proposal submitted to Jackson & Tull/Air Force Research Laboratory which was awarded $180,000.

**17. Development of an Unstructured Grid Algorithm for Turbomachinery**

- PI: Dr. Kidambi Sreenivas, UT SimCenter at Chattanooga
- Develop an algorithm capable of numerically simulating the flow field arising from multi-row (purely axial, as well as axial and radial combinations) turbomachinery. This algorithm will be implemented in an unstructured flow solver as unstructured grids are inherently more capable of handling complex geometries than corresponding structured grids. This capability will be used to carry out simulations of the unsteady interactions between blade rows of a turbomachine. This capability can also be applied to carry out simulations of a class of problems that involve rotation about a fixed axis, for example, propellers attached to ships and submarines, tilt-rotor aircrafts, helicopter rotor blades undergoing cyclic pitch variation etc.
- Results: Dr. Sreenivas' work contributed to the following proposals for external funding which were funded for total of $2,583,072.

- A proposal submitted to NASA Glenn Research Center which was awarded $1,527,072 over three years.
- A proposal submitted to the Office of Naval Research which was awarded $1,056,000.

*Completed Research Activities Funded by the Center in Fiscal Year 2005-2006*

**1. Numerical Solution of the Boltzmann Equation with BGK Approximation**

- PI: Mr. R. Glenn Brook, UT SimCenter at Chattanooga
- Develop a robust solution algorithm and parallel computer code for numerically solving the Boltzmann equation with one or more variants of the Bhatnagar-Gross-Krook (BGK) collision model. This work will serve as a foundation for future research into multispecies flows, chemically reactive flows, plasma flows, combustion, and computational design of nanoscale devices.
- Results: Mr. Brook submitted a white paper to the Army Research Laboratory in April 2006. The white paper was accepted and a full proposal was submitted in June 2006. The proposal was not funded. Mr. Brook submitted a pre-application to the Department of Energy in July 2006. The pre-application was not selected for submission as a full proposal.

Summary of CEACSE funding allocation (Figure 2) illustrates the major categories of to which the CEACSE budget was allocated for Center activities during its first two years of operation.

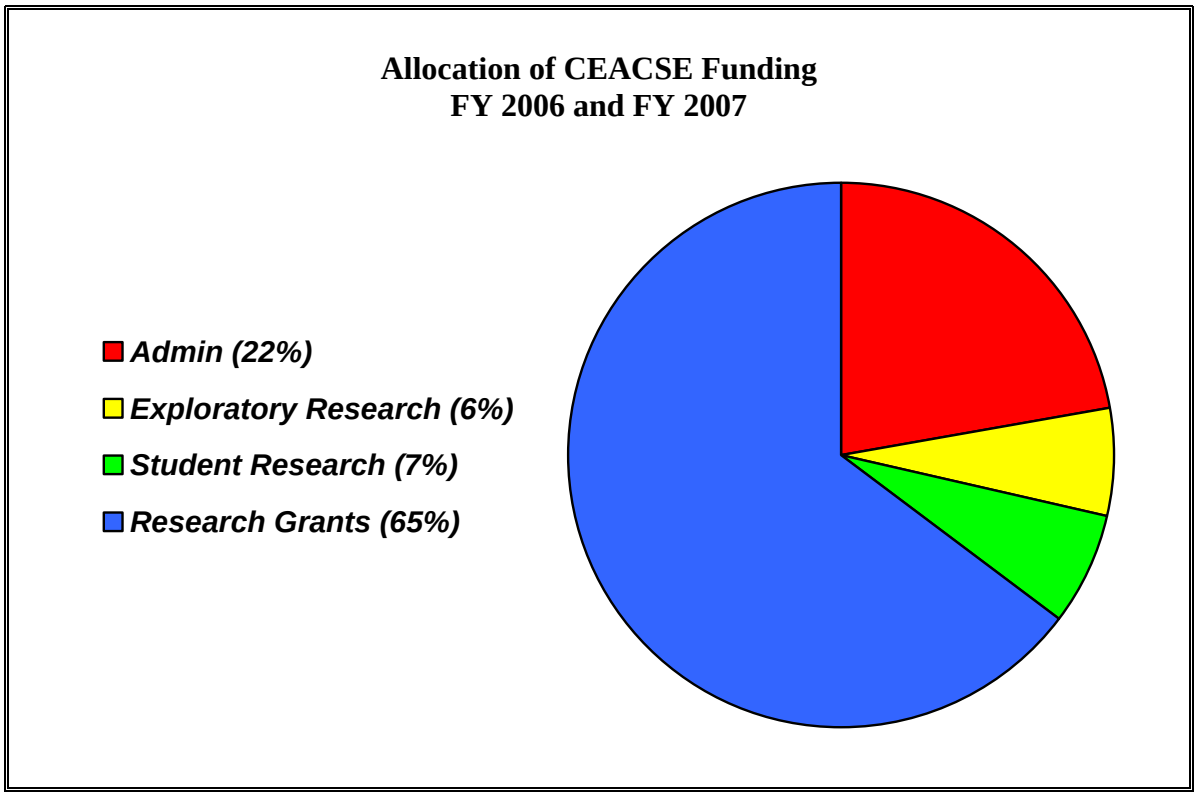



**Figure 2**

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

| | |
|---|---|
| External Funding Awarded in Fiscal Year 2005-2006: | $2,195,529** |
| External Funding Awarded in Fiscal Year 2006-2007: | $3,291,102 |
| **Total External Funding Awarded:** | **$5,486,631** |

_____

* These funds represent funds committed by external funding agencies. Some of the awards included are multi-year awards with each year's funding dependant upon availability of funds.
** The funding amount of two awards reported in the previous annual report as pending were reduced upon receipt.

***Results of FY 2006 Proposals Submitted for External Funding***

1. National Aeronautics and Space Administration
    a. Proposal not funded
    b. Title: Computational/Experimental Evaluation of Flow Control Concepts for Compressor Stall Mitigation
    c. Associated CEACSE grants:
        i. Development of an Unstructured Grid Algorithm for Turbomachinery; Dr. Kidambi Sreenivas
        ii. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman
        iii. Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III

iv. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams

v. Computational Methods for Field Simulations; Dr. W. Roger Briley

2. National Aeronautics and Space Administration

   a. Proposal not funded

   b. Title: Rotorcraft Small Engine Compressor Stall Analysis

   c. Associated CEACSE grants:

      i. Development of an Unstructured Grid Algorithm for Turbomachinery; Dr. Kidambi Sreenivas

      ii. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman

      iii. Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III

      iv. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams

      v. Computational Methods for Field Simulations; Dr. W. Roger Briley

3. National Aeronautics and Space Administration

   a. Proposal funded

   b. Funding Awarded: $700,674

c. Title: A Generalized Framework for Constrained Design Optimization of General Supersonic Configurations Using Adjoint Based Sensitivity Derivatives

d. Associated CEACSE grants:

i. Geometry Manipulation and Visualization, Computational Simulation and Design; Ms. Dawn Ellis, Dr. Steve Karman

ii. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman

iii. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams

4. Army Research Office

a. Proposal not funded

b. Title: Computational Design of Catalytic Surfaces with Nanoscale Features

c. Associated CEACSE grants:

i. Numerical Solution of the Boltzmann Equation with BGK Approximation; Mr. R. Glenn Brook

5. Department of Energy

a. Preapplication not selected

b. Title: Computational Design of Catalytic Surfaces with Nanoscale Features

c. Associated CEACSE grants:

i. Numerical Solution of the Boltzmann Equation with BGK Approximation; Mr. R. Glenn Brook

6. Office of Naval Research
    a. White Paper not selected
    b. Title: Adjoint Method for Solid Oxide Fuel Cell Simulations
    c. Associated CEACSE grants:
        i. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman
        ii. Computational Analysis and Design of Fuel Cell Components; Dr. W. Kyle Anderson, Dr. Steve Karman
7. Office of Naval Research
    a. Proposal funded
    b. Funding Awarded: $1,584,000
    c. Title: Unstructured Viscous Free Surface Solver for Predicting Hydrodynamic Performance of High Speed Ships
    d. Associated CEACSE grants:
        i. Evaluation and Enhancement of an Unstructured Grid Algorithm for Free Surface; Dr. Robert Wilson
        ii. Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III
        iii. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams

iv. Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers; Dr. Ramesh Pankajakshan

v. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman

vi. Development of an Unstructured Grid Algorithm for Turbomachinery; Dr. Kidambi Sreenivas

8. American Chemical Society, Petroleum Research Fund

   a. Proposal not funded

   b. Title: A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysis in Microchannels

   c. Associated CEACSE grants:

      i. A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysts; Dr. Frank Jones

9. Defense Threat Reduction Agency

   a. Whitepaper not funded

   b. Title: Particulate and Agent Dynamics in Multiphase Turbulent Reacting Flows

   c. Associated CEACSE grants:

      i. Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III

10. Radiance Technologies
    a. Proposal funded
    b. Funding Awarded: $250,000
    c. Title: Algorithms for Simulation of Electromagnetically Large Structures
    d. Associated CEACSE grants:
        i. Computational Methods for Field Simulations; Dr. W. Roger Briley
        ii. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams
        iii. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman
11. Science and Technology Applications, LLC
    a. Proposal funded
    b. Funding Awarded: $25.356
    c. Title: Analytical Modeling of Liquid Rocket Instability
    d. Associated CEACSE grants:
        i. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman

12. Aerotonomy, Inc.
    a. Proposal funded
    b. Funding Awarded: $25,000
    c. Title: Computational Analysis of Synthetic Jet Actuators Supporting Aerotonomy, Inc.
    d. Associated CEACSE grants:
        i. Computational Methods for Field Simulations; Dr. W. Roger Briley
13. Coronal Energy, LLC
    a. Proposal funded
    b. Funding Awarded: $192,000
    c. Title: Plasma-Dynamics Software Interface and Test Cases
    d. Associated CEACSE grants:
        i. Computational Methods for Field Simulations; Dr. W. Roger Briley
        ii. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams
        iii. Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers; Dr. Ramesh Pankajakshan
        iv. Adjoint Method for Magnetohydrodynamic Simulations; Dr. W. Kyle Anderson, Dr. Steve Karman

e. Correction to FY 2006 Annual Report: Dr. Daniel Hyams and Dr. Kyle Anderson were incorrectly listed as contributing to this external grant.

14. Jackson & Tull/Air Force Research Laboratory

a. Proposal funded

b. Funding Awarded: $180,000

c. Title: Computational Modeling and Simulation Tools for Solid Rocket Motor (SRM) Analysis and Design

d. Associated CEACSE grants:

i. Advancement and Verification of the Navier-Stokes Flow Solver for Rocket Motor; Dr. Abdollah Arabshahi

***Results of FY 2007 Proposals Submitted for External Funding***

1. National Aeronautics and Space Administration

a. Proposal funded

b. Funding Awarded: $1,527,072

c. Title: Validated Aerodynamic Analysis and Design Tools for Integrated Embedded Propulsion Systems

d. Associated CEACSE grants:

i. Extensible Adjoint Method for Sensitivity Analysis, Error Estimation and Adaptive Meshing; Dr. Kyle Anderson, Dr. Steve Karman

ii. Geometry Manipulation and Visualization, Computational Simulation and Design; Dr. Kyle Anderson, Dr. Steve Karman

iii. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams

iv. Development of an Unstructured Grid Algorithm for Turbomachinery; Dr. Kidambi Sreenivas

v. Computational Methods for Field Simulations; Dr. Roger Briley

2. Aerospace Alliance Testing

   a. Proposal funded

   b. Funding Awarded: $25,000

   c. Title: Analysis of Total Temperature Measurement Correction Techniques in the Aerodynamic and Propulsion Test Unit (APTU)

   d. Associated CEACSE grants:

      i. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams

      ii. Computational Methods for Field Simulations; Dr. Roger Briley

3. The Enterprise Center/ Small Business Administration

   a. Proposal funded

   b. Funding Awarded: $456,529

   c. Title: TEC Chattanooga Fuel Cell Demonstration

   d. Associated CEACSE grants:

      i. Computational Analysis and Design of Fuel Cell Components; Dr. W. Kyle Anderson, Dr. Steve Karman

      ii. Computational Engineering with Solid Oxide Fuel Cells; Dr. James Henry

4. Defense Threat Reduction Agency
    a. Proposal not funded
    b. Title: Dependable Information Communication System (DICS) in Disaster Management
    c. Associated CEACSE grants:
        i. Information Communication Mediator Model in Disaster Management; Dr. Li Yang and Dr. Joseph Kizza
5. Oak Ridge National Laboratory
    a. Proposal not funded
    b. Title: Dependable Communication System (DCS) in Disaster Management
    c. Associated CEACSE grants:
        i. Information Communication Mediator Model in Disaster Management; Dr. Li Yang and Dr. Joseph Kizza
6. National Science Foundation
    a. Proposal not funded
    b. Title: Project EPIC: Expanding Participation in Computing of Low Income Single Mother Families Through Inquiry Learning
    c. Associated CEACSE grants:
        i. Information Communication Mediator Model in Disaster Management; Dr. Li Yang and Dr. Joseph Kizza
7. National Science Foundation
    a. Proposal not funded

b. Title: Project CSI (Computer Science Investigations): Increasing Female and Minority Participation in Information Technology

c. Associated CEACSE grants:

   i. Information Communication Mediator Model in Disaster Management; Dr. Li Yang and Dr. Joseph Kizza

***FY 2007 Publications and Presentations of the Center's Research Activities***

1. Wang, J., Batelaan, H., Podany, J. and Starace, A.F., "Entanglement evolution in the presence of decoherence", *Phys. B: At. Mol. Opt. Phys.*, Vol. 39 No 21, 14 November 2006, pp. 4343-4353.
2. S. Kapadia , W.K. Anderson, L. Elliott, C. Burdyshaw, "Adjoint method for solid-oxide fuel cell simulations", *Journal of Power Sources*, Vol. 166, 2007, pp. 376-385.
3. S. Kapadia, W. K. Anderson and L. Elliott, "Design and Sensitivity Analysis of Solid Oxide Fuel Cells Using Discrete Adjoint Method", 5th International Energy Conversion Engineering Conference and Exhibit (IECEC), 25 - 27 June 2007, St. Louis, Missouri, AIAA 2007-4832.
4. S. Kapadia, W. K. Anderson, L. Elliott and C. Burdyshaw, "Adjoint Based Sensitivity Analysis And Error Correction Methods Applied To Solid Oxide Fuel Cells", Presented at ASME 5th International Fuel Cell Science, Engineering & Technology Conference, June 18 - 20, 2007, New York, FuelCell 2007-25157.

5. Carrica, P., Wilson R., and Stern F., “An Unsteady Single-Phase Level Set Method for Viscous Free Surface Flows,” Vol. 53, No. 2, *Int. J. of Num. Methods Fluids* , Jan. 2007, pp. 229-256.
6. A. Arabshahi, K. Sreenivas, S. Nichols, B. Mitchell, L. Taylor and D. Whitfield, "Computational Analysis of Turbulent Internal Flow in Ballistic Rocket Motors," AIAA-2007-1449, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
7. Karman Jr., S.L., and Sahasrabudhe, M., "Unstructured Adapted Elliptic Smoothing," AIAA-2007-0559, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
8. Karman Jr., S.L., Mitchell, B., Sawyer, S., Whitt, J., "Unstructured Grid Solutions of CAWAPI F-16XL by UT SimCenter," AIAA-2007-0681, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
9. K. Sreenivas, S. Nichols, D. Hyams, B. Mitchell, S. Sawyer, and D. Whitfield, "Computational Simulation of Heavy Trucks," AIAA-2007-1087, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
10. K. Sreenivas, B. Mitchell, S. Sawyer, S. Karman, S. Nichols, and D. Hyams, "Computational Prediction of Forces and Moments for Transport Aircraft," AIAA-2007-1088, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
11. Pankajakshan, R., Mitchell, B.J., and Taylor, L.K., "Simulation of Unsteady Two-Phase Flows using a Parallel Eulerian-Lagrangian Approach," AIAA-2007-0340,

45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.

12. S. Nichols, K. Sreenivas, S. Karman and B. Mitchell, "Turbulence Modeling for Highly Separated Flows," AIAA-2007-1407, 45th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 8-11, 2007.
13. Wilson R., Carrica, P., and Stern F., "Simulation of Ship Breaking Bow Waves and Induced Vortices and Scars," in press and available online, DOI: 10.1002/FLD.1406, *Int J. Num. Methods Fluids*, Jan. 2007.
14. S. Karman Jr., "Unstructured Viscous Layer Insertion Using Linear-Elastic Smoothing," AIAA Journal, Volume 45, Number 1, pp. 168-180, January 2007.
15. Tahara Y., Wilson R., Carrica, P., and Stern F., "RANS Simulation of a Container Ship Using a Single-Phase Level Set Method with Overset Grids and the Prognosis for Extension to Self-Propulsion Simulator," Vol. 11, No. 4, 2006, pp. 209-228.
16. Almeida, T.G., Walker, D.T., Leighton, R.I., Alajbegovic, A., Pankajakshan , R., Taylor, L.K., Whitfield, D.L., Ceccio, S.L., “A Reynolds-Averaged Model for the Prediction of Friction Drag Reduction by Polymer Additives,” 26th Symposium on Naval Hydrodynamics, Rome Italy, September. 17-22, 2006.
17. Carrica, P.M., Wilson, R.V., Noack, R., Xing, T., Kandasamy, M., Shao, J., Sakamoto, N., Stern, F., “A Dynamic Overset, Single-Phase Level Set Approach for Viscous Ship Flows and Large Amplitude Motions and Maneuvering,” 26th Symposium on Naval Hydrodynamics, Rome Italy, September. 17-22, 2006.

18. Wilson, R.V., Nichols, D.S., Mitchell, B., Karman, S.L., Hyams, D.G., Sreenivas, K., Taylor, L.K., Briley, W.R., and Whitfield, D.L., "Application of an Unstructured Free Surface Flow Solver for High Speed Transom Stern Ships," 26th Symposium on Naval Hydrodynamics, Rome Italy, September. 17-22, 2006.

19. Arabshahi, A., Webster, R. S., Briley, W. R., and Whitfield, D. L., "Numerical Analysis of Solid Propellant Rocket Motor Internal Flows," AIAA-2006-5114, July, 2006.

20. Hixson, J., Potter, J., and Henry, J., "Chattanooga Fuel Cell Demonstration Project", American Institute of Chemical Engineers Annual Meeting, San Francisco CA, November 2006.

21. Lange, K.J., "A Fully Implicit Characteristic-Based Algorithm for a One Dimensional Radio Frequency Glow Discharge Fluid Simulation", Masters Thesis, University of Tennessee at Chattanooga, August 2007.

22. N. Alp, F. Jones, R. Bailey, and J. Hiestand, "Conversion Rate Optimization in Biomicroreactors Using the Taguchi Method," Institute of Industrial Engineers Annual Conference, May 2007, Nashville, TN.

23. S. Wilson and F. Jones, "The Effects of Micromixing on heterogeneous Catalysis in Microbioreactor Channels," ASEE Southeastern Section Conference, Louisville, KY, April 1-3, 2007.

24. S. Wilson and F. Jones, "The Effects of Micromixing on Heterogeneous Catalysis in Microbioreactor Channels," AIChE Annual Meeting, San Francisco, CA, November 11-15, 2006. Stephanie Wilson won a 2nd place award for this presentation in an undergraduate student research competition, Biotech Division.

25. F. Jones, R. Bailey, S. Wilson, and J. Hiestand, "The Effects of Engineering Design on Heterogeneous Catalysis in Microchannels." 28th Symposium on Biotechnology for Fuels and Chemicals, Nashville, TN, May 2006.

26. N. Alp, F. Jones, R. Bailey, and J. Hiestand "The Use of Taguchi Statistical Methods to Optimize the Design of Biomicroreactors." Institute of Industrial Engineers Annual Conference, Orlando, FL, May 2006.

27. R. Bailey, F. Jones, S. Wilson, S. Ryan, and J. Hiestand, "The Effects of Packing Patterns on Mixing and Heterogeneous Catalysis in Microchannels," 2007 ASME Fluids Engineering Conference Symposium Series (peer-reviewed), July 29-August 2, 2007, San Diego, CA.

28. F. Jones, R. Bailey, S. Wilson, and J. Hiestand, "The Effects of Engineering Design on Heterogeneous Biocatalysis in Microchannels." Applied Biochemistry and Biotechnology, Vol. 136-140, 115-129 (2007).

29. Stephanie Wilson and Frank Jones, "A Study of the Effects of Various Flow Obstructions on Heterogeneous Catalysis and Micromixing in Biocatalytic Microchannels," Analytical Sciences Digital Library, eUndergraduate Research Online Journal, March 2007. http://www.asdlib.org/eUGHUploads/45_eUGH_publication.pdf?PHPSESSID=63458ea223f63d9a15ee548ed6a3a01a.

30. Alp, N.; Jones, F.; Bailey, R.; and Hiestand, J.; "Use of Taguchi Methods to Optimize the Design of Biomicroreactors," Institute of Industrial Engineers (IIE) Annual Conference Proceedings, pp. 108-113, May 20-24, 2006, Orlando, FL.

31. Wilson, S., "A Study of the Effects of Various Flow Obstructions on Heterogeneous Catalysis and Micromixing in Biocatalytic Microchannels", Undergraduate honors thesis, 2007.

32. L. Elliott, W. K. Anderson, S. Kapadia, and C. Burdyshaw, "Analysis and Design of Solid Oxide Fuel Cells with Advanced Numerical Techniques", AIAA 5th International Energy Conversion Engineering Conference and Exhibit, 25 - 27 June 2007, St. Louis, Missouri, AIAA 2007-4834.

33. L. Elliott, W. K. Anderson, and S. Kapadia, "Solid Oxide Fuel Cell Design Optimization with Numerical Adjoint Techniques", Presented at ASME 5th International Fuel Cell Science, Engineering & Technology Conference, June 18 - 20, 2007, New York, FuelCell2007-25313.

Burdyshaw, C. E., Anderson, W. K., Lange, K., "Advances in Discrete Sensitivity Methods Applied to Uncertainty Analysis," NATO AVT-RTO-147 Meeting on Computational Uncertainty in Military Vehicle Design. Athens, Greece. To be presented Dec 7, 2007.

## Conclusion

CEACSE has established operations and is positioned to continue to enhance and expand research and assist in the obtaining of external funding opportunities. Research funding for a number of diverse projects has engaged more faculty and students across the campus. The committed seed funding enabled various faculty to pursue their research and develop opportunities to obtain follow-on support externally. The Center has a requirement for recipients of funding to submit proposals to a credible agency and/or

company which have an interest in the research being conducted. As evidenced, there is already a growing level of external funding being secured from the activities of the Center. This should continue into the future.

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

Through the seed funding for research activities, undergraduate and graduate students are being engaged in a diverse range of topics. Additional efforts in this area assist in increasing the interaction and involvement of students with research faculty. Additional efforts will need to be defined, focused, and initiated to enhance/increase outreach to pre-college students. This area needs additional and continued attention. Hopefully these efforts when combined with other external activities in the field will lead to stimulated interest in science and engineering.

THE UNIVERSITY OF TENNESSEE
SimCenter
AT CHATTANOOGA
Computational Simulation and Design Center
GRADUATE SCHOOL OF COMPUTATIONAL ENGINEERING

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL
SCIENCE AND ENGINEERING

***Advisory Board***

23 September 2008

Dr. Henry McDonald
Director
Tennessee Higher Education Commission
Center of Excellence in Applied Computational Science and Engineering
701 East M. L. King Boulevard
Chattanooga, TN 37403

Dear Dr. McDonald,

On behalf of myself and the rest of the advisory board, let me thank you and the other personnel at University of Tennessee at Chattanooga, UTC, for the excellent program reviews and meetings with various groups provided on September 17 and 18, 2007. This was the third meeting of the board to review the THEC Center at UTC, and the SimCenter. Since our last meeting, the board has seen the THEC Center mature into a positive force in the development of increased research efforts and external research funding at UTC. With limited time, the board was only able to briefly look over the SimCenter operation, but all seems well with all goals in terms of students, graduations, research programs, and funding being met or exceeded. The presentation of plans to expand the SimCenter into a National Center for Computational Engineering were well received and strongly endorsed by the board.

The advisory board's findings are enclosed in briefing chart form. If you have questions or need any clarification on the enclosed material please contact myself or any of the other board members as needed.

Sincerely,

Eric R. McFarland

Eric R. McFarland

# Program Review Board Report

*THEC/SimCenter Advisory Board* *September 17-18, 2007*

**Debriefing of the Meeting of the Advisory Board**
**of the Graduate School of Computational Engineering,**
**the SimCenter,**
**and the THEC COE in Applied Computational Science & Engineering**
**at the University of Tennessee, Chattanooga**
**17-18 September 2007**

Advisory Board Members: Dale Anderson, C. T. Cozart, Jim Fein,
David Keyes, Eric McFarland, Bill Stacey

We thank:
SimCenter Leaders Henry McDonald, Dave Whitfield, Roger Briley,
Tim Swafford

Members of the Foundations, RiverCity, and Enterprise Center

Roger Brown, UTC Vice Chancellor of Finance, Phil Oldham, Provost
Jim Cunningham Dean of Engineering

Dr. Dan Stewart of the UT System

And All the SimCenter and UTC Folks for their warm hospitality.

*THEC/SimCenter Advisory Board* *September 17-18, 2007*

**THEC COE in Applied Computational Science & Engineering Review**

Positives

Projects selected thus far have given excellent return on investment

Nice cross section of projects funded. All seem related to COE mission in applied computational science and engineering

Good effort to bring in and make use of faculty and students through out UTC

Addition of vice provost for research position

Negatives

Lack of desire or ability of non-SimCenter personnel to propose research efforts at UTC. Some sort of educational effort or incentive (withholding of tenure) may be required to change culture concerning pursuit of research grants

Need to fill Dean of Engineering post. Candidates should have strong interest and some expertise in developing a strong research efforts throughout UTC

Tennessee Higher Education Commission

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA

# CENTER OF EXCELLENCE

# IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

*Established July 1, 2005*

## Report to Advisory Board

*Activities for FY 2005-2007*

Dr. Henry McDonald, *Director*

*September 17, 2007*

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

### Strategic Goal

Recognition as a National Center of Excellence and Premier Multidisciplinary Research and Education Center for Computational Science and Engineering

### Research Focus

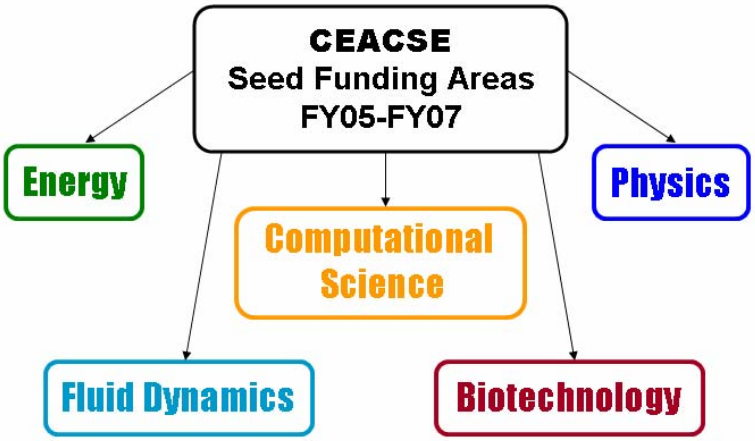
New programs to collectively advance state-of-the-art in computational simulation

### Computational Approach

Computational Expertise (SimCenter) + Discipline experts = Seeded Research success

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

## Topical Areas Funded




THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

## Objectives

1. Expand capabilities of the University in computational science & technology and seed research and educational activities
2. Increase participation of faculty, graduate and undergraduate students in computational based R & D
3. Directly and indirectly support economic develop initiatives that benefit State of Tennessee

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

## Summary

***CEACSE Seed Funding Committed for Research Activities***

| | Project | FY05-07 | Students Used | Externally Funded | |
|---|---|---|---|---|---|
| Comp. Science | Computational Methods for Field Simulations | 166,445 | | Coronal Energy, Aerospace Testing, Aerotonony, NASA Glenn, Radiance | |
| | Computation of Dynamic Stability and Control Devices | 166,250 | | | |
| | Computational Analysis and Design of Fuel Cell Components | 124,329 | ● | The Enterprise Center/Small Business Admin. | |
| | Information Communication Mediator Model in Disaster Management | 33,250 | | | * |
| | Multiprocessor Objective-C Computer Systems for HPC | 61,200 | ● | | * |
| Ph Bio | A Fund. Study of the Eff. of Dos. on Heterogeneous Biocatalysts | 37,870 | | | * |
| Ph | Quantum Measurement and Feedback in Atomic Systems | 18,420 | | | * |
| Fluid Dynamics | Geometry Manipulation & Visualization, Comp. Sim. & Des. | 59,109 | ● | NASA Langley, NASA Glenn | |
| | Advanced Turbulence Modeling for Unstructured Topologies | 166,056 | | Department of Energy, Office of Naval Research | |
| | Uns.Sol. Alg. Sys. Int., Des.&Test. | 66,550 | | Department of Energy, Office of Naval Research, Aerospace Testing Alliance, NASA Glenn | |
| | Eval. and Enhance. of an Unstructured Grid Algorithm for Free Surface | 116,160 | | Office of Naval Research | |
| | Development of an Unstructured Grid Algorithm for Turbomachinery | 98,318 | ● | Office of Naval Research, Aerotonomy, NASA Glenn | |
| | Ext. Adjoint Meth. for Sens. Anal., Error Est. ,& Adapt. Mesh. | 148,298 | ● | Office of Naval Research, Science & Technology Applications, NASA Langley, NASA Glenn | |
| | Adv. and Ver. of the Navier-Stokes Flow Solver for Rocket Motor | 100,078 | | Science & Technology Applications, Jackson & Tull/Air Force Research Laboratory | |
| | Numerical Solution of the Boltzmann Equation with BGK Approximation | 160,100 | ● | | |
| Energy | Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers | 96,255 | | Office of Naval Research, Riverbend Technology Institute, Jackson & Tull/Air Force Research Lab | |
| | Adjoint Method for Magnetohydrodynamic Simulations | 95,391 | ● | Coronal Energy | |
| | Computational Engineering with Solid Oxide Fuel Cells | 110,000 | ● | The Enterprise Center/Small Business Admin. | * |

* *Researchers external to SimCenter*

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

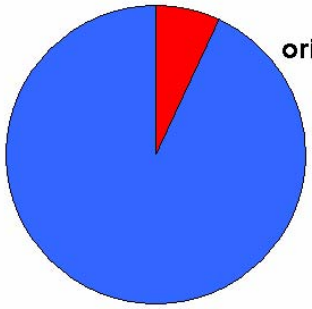
## External Funding FY05-FY07

***Directly and Indirectly the Result of CEACSE Fund***

| | |
|---|---|
| Department of Energy | $4,002,750 |
| Office of Naval Research | $1,056,000 |
| Radiance Technologies | $ 450,000 |
| Science and Technology Applications, LLC | $ 25,356 |
| Coronal Energy | $ 192,000 |
| Jackson & Tull/Air Force Research Laboratory | $ 300,000 |
| Small Business Administration/The Enterprise Center | $ 456,529 |
| NASA Langley | $ 700,674 |
| NASA Glenn | $1,527,072 |
| Aerotonomy | $ 75,000 |
| Aerospace Testing Alliance | $ 65,000 |
| SPARTA, Inc. | $ 210,000 |
| Barber-Nichols, Inc. | $ 190,000 |
| ITT Industries | $ 100,000 |

THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

## Funding Allocation

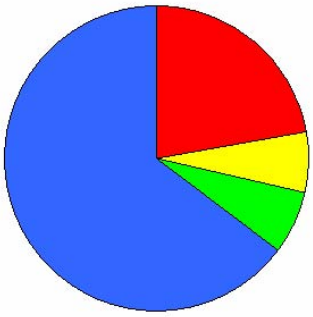


**External Funding originating from seed projects FY 06 and FY 07**

- *Admin and Exploratory Research (7%)*
- *Student Research (0%)*
- *Research Grants (93%)*

**CEACSE Funding (FY 06 and FY 07)**

- *Admin (22%)*
- *Exploratory Research (6%)*
- *Student Research (7%)*
- *Research Grants (65%)*



THE UNIVERSITY OF TENNESSEE AT CHATTANOOGA
CENTER OF EXCELLENCE
IN APPLIED COMPUTATIONAL SCIENCE AND ENGINEERING

## Faculty and Students Utilized

| | | *FY05-06* | *FY06-07* |
|---|---|---|---|
| | **Faculty** | 17 | 17 |
| *Students* | **PhD** | 8 | 7 |
| | **Masters** | 11 | 13 |
| | **Undergraduate** | 5 | 8 |

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## The Way to the Future

***(where no computational engineer has gone before)***

- Strengthen Base in CFD
- Continue Electromagnetics and Alternative Energy Support
- Initiate Remote Agent Research
- Support Solid Mechanics (Lifing new hire)
- Other opportunities?

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## Major Issues

- Hiring and Succession Planning
- Convince THEC to increase annual funding
- Poor non-SimCenter based participation

**Dr. Eric McFarland**
mcflnd@cox.net

Dr. Eric McFarland is a retired Aerospace Engineer from the Propulsion Group at NASA Lewis Research Center. He is currently teaching at Cuyahoga Community College in Cleveland Ohio and is an Advisory Board member for the Tennessee Higher Education Commission Center of Excellence in Computational Science and Engineering and the University of Tennessee SimCenter at Chattanooga. His areas of expertise include Aerodynamics, Aerodynamics of Turbomachinery, Aerodynamic Design of Turbomachinery, and Computational Fluid Mechanics. Dr. McFarland receive is Ph.D. in Aerospace Engineering in 1976 at the University of Cincinnati.

**C.T. Cozart, Jr.**
ctcozart@comcast.net

Mr. C.T. Cozart, Jr. retired from the Chevron Corporation in 1997. He was Vice President of Marketing for Global Lubricant from 1989 to 1997 and was responsible for sales and marketing worldwide, traveling to over 65 foreign countries, managing hundreds of employees and managing the bottom line profit and loss. He holds a Bachelor of Science degree from the College of Business, University of Tennessee, Knoxville, majoring in marketing. He has logged over one hundred additional classroom hours in the Customer Value Institute at UTK with a thesis on New Product Development.

He is Chairman of the Board of Trustees for Carson-Newman College, Advisory Board member for the Tennessee Higher Education Commission Center of Excellence in Computational Science and Engineering and the University of Tennessee SimCenter at Chattanooga, President of CCC Enterprises, Inc. and past board member of numerous industry related companies. He is a frequent speaker at various civic and professional functions and active in church and denominational activities.

**Dr. Dale A. Anderson**
daymar@suddenlink.net

Dr. Dale Anderson, Professor Emeritus, Aerospace Engineering, The University of Texas at Arlington received his Ph.D. in Aerospace Engineering and Electrical Engineering from Iowa State University in 1964. He began his career in 1957 as a graduate assistant at Iowa State University while working on his Masters, spending the summers as Flight Test Engineer for Douglas Aircraft Co. in Santa Monica, California, an Aerodynamicist for Boeing Airplane Co. in Wichita, Kansas and a Technical Staff Member for Aerospace

Corporation in El Segundo, California. In 1961 he became an assistant Professor of Aerospace Engineering at Iowa State University, promoted to Associate Professor in 1965 and Full Professor in 1975. He was Director of the Computational Fluid Dynamics Institute from 1980 to 1984 at which time he took a position as Professor of Aerospace Engineering at the University of Texas at Arlington. While at UT Arlington he became Associate Dean for Research for the College of Engineering in 1996, Vice President for Research and Dean of Graduate Studies in 1997 and Vice President for Research and Vice President, UTA/Fort Worth - Riverbend Campus in 2000 continuing that position until 2002. He gained Professor Emeritus status in 2006.

Dr. Anderson has consulted with numerous corporations such as Standard Oil Production Co./British Petroleum, General Dynamics Corporation, Lockheed-Martin Corporation, Lockheed Research Laboratory, Union Carbide Corporation, General Electric Corporation, Rockwell International, and the United States Air Force-Army Research Laboratory.

## Dr. David Keyes

kd2112@columbia.edu

David Keyes is a computational mathematician with primary interests in parallel numerical algorithms and large-scale simulations of transport phenomena ─ fluids, combustion, and radiation. He is currently the Acting Director of the Institute for Scientific Computing Research (ISCR) at Lawrence Livermore National Laboratory. Dr. Keyes is also the Fu Foundation Professor of Applied Mathematics in the Department of Applied Physics and Applied Mathematics at Columbia University and serves on the advisory board to the University of Tennessee SimCenter at Chattanooga and the Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering.

Dr. Keyes is active in the Society of Industrial and Applied Mathematics (SIAM) and in the domain decomposition, parallel CFD, and petaflops architecture research communities. He earned a Bachelor's degree in Mechanical Engineering (BSE) at Princeton in 1978, and a Ph.D. in Applied Mathematics at Harvard in 1984. Dr. Keyes also served a s post-doctoral fellow in the Computer Science Department at Yale in 1984-1985. He has directed an NSF Grand Challenge center and an ASCI Level-2 center and is now directing an Integrated Software Infrastructure Center in DOE's Scientific Discovery through Advanced Computing Initiative, called Terascale Optimal PDE Simulations. He is the editor-in-chief of the 2003 DOE report "A Science-based Case for Large-scale Simulation."

## Dr. Bill Stacy

bill_stacy@baylorschool.org

Dr. Stacy holds a Bachelor of Science degree from Southeast Missouri State University, where he was later president for ten years, a Masters in Speech Communication and a Doctorate in Contemporary Address and Communication Theory from Southern Illinois University.

Stacy moved to Tennessee after serving as a Founding President of one of the California State University campuses in a system of over 300,000 students. In eight years at California State University San Marcos, Stacy was able to see immediate action to a strategic plan that involved creating the unique portions of mission and purpose, recruiting faculty and staff, designing and building not only the academic plan – but the buildings and student body as well. Prior to the unusual experience in California, Stacy had served a ten-year presidency at Southeast Missouri State University, his alma mater.

Bill was Chancellor of UTC from 1997 until 2004. During his tenure at UTC, Bill oversaw the largest capital growth in the institution's history – $200 million worth of projects that included a new Engineering, Math, and Science Building, an expanded university center, and new residence halls – as well as the creation of three doctoral programs.

Currently Dr. Stacy is only the eighth headmaster in 111-years for the Baylor School in Chattanooga. He also serves on the Advisory Board for the University of Tennessee SimCenter at Chattanooga and the Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering.

## James A. Fein

fein123@comcast.net

Jim Fein bid farewell to Naval Surface Warfare Center, Carderock Division after two years as its Executive Director in April of 2003. With 34 years of service, he ended his Federal career where it began.

Fein's first position with the Federal government began in 1969 as a naval architect with the Naval Ship Research and Development Center. Over his 30+ years of service he has worked for the Office of the Deputy Assistant Secretary of the Navy for Research and Advanced Technology, the Office of Naval Research, and the Naval Sea Systems Command. He was also a visiting professor at Defense Systems Management College.

Fein has received two *Navy Superior Civilian Service Awards*, one from NAVSEA and one from ONR. He holds a bachelor's degree in applied mechanics from the University of Michigan (1969) and a master's degree in mechanical engineering from the University of Maryland (1972).

Mr. Fein is currently working part-time as a consultant and serves on the Advisory Board for the University of Tennessee SimCenter at Chattanooga and the Tennessee Higher Education Commission Center of Excellence in Applied Computational Science and Engineering.

**Schedule 7**

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

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

| | FY 2006-07 Actual | | | FY 2007-08 Proposed | | | FY 2008-09 Requested | | |
|---|---|---|---|---|---|---|---|---|---|
| | Matching | Appropr. | Total | Matching | Appropr. | Total | Matching | Appropr. | Total |
| Expenditures | 357,578 | 817,300 | **1,174,878** | 357,578 | 832,800 | **1,190,378** | 357,578 | 874,440 | **1,232,018** |
| **Salaries** | | | | | | | | | |
| Faculty | 166,535 | 388,581 | **555,116** | 235,583 | 549,695 | **785,278** | 199,264 | 487,852 | **687,116** |
| Other Professional | 31,447 | 73,377 | **104,824** | 31,447 | 73,377 | **104,824** | 30,399 | 74,425 | **104,824** |
| Clerical/ Supporting | 3,345 | 7,806 | **11,151** | 3,345 | 7,806 | **11,151** | 3,234 | 7,917 | **11,151** |
| Assistantships | 63,434 | 148,012 | **211,445** | 63,434 | 148,012 | **211,445** | 61,319 | 150,126 | **211,445** |
| **Total Salaries** | **264,761** | **617,775** | **882,536** | **333,809** | **778,889** | **1,112,698** | **294,215** | **720,321** | **1,014,536** |
| **Longevity** | | | | | | | | | |
| **Fringe Benefits** | 51,348 | 119,812 | **171,160** | 67,140 | 156,661 | **223,801** | 53,680 | 131,423 | **185,103** |
| **Total Personnel** | **316,109** | **737,587** | **1,053,696** | **400,950** | **935,549** | **1,336,499** | **347,895** | **851,744** | **1,199,639** |
| **Non-Personnel** | | | | | | | | | |
| Travel | 5,883 | 13,728 | **19,612** | 6,544 | 15,268 | **21,812** | 5,687 | 13,924 | **19,612** |
| Software | | | **0** | | | **0** | | | **0** |
| Books & Journals | 158 | 370 | **528** | 158 | 370 | **528** | 158 | 370 | **528** |
| Other Supplies | 1,585 | 3,699 | **5,284** | 14,744 | 34,402 | **49,145** | 1,585 | 3,699 | **5,284** |
| Equipment | | | **0** | | | **0** | | | **0** |
| Maintenance | | | **0** | | | **0** | | | **0** |
| Scholarships | 2,087 | 4,869 | **6,955** | 15,836 | (7,382) | **8,454** | 2,252 | 4,704 | **6,955** |
| 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** | **9,714** | **22,665** | **32,379** | **37,281** | **42,658** | **79,939** | **9,683** | **22,696** | **32,379** |
| **GRAND TOTAL** | **325,823** | **760,253** | **1,086,075** | **438,231** | **978,207** | **1,416,438** | **357,578** | **874,440** | **1,232,018** |
| **Revenue** | | | | | | | | | |
| New State Appropriation | | 817,300 | **817,300** | | 832,800 | **832,800** | | 874,440 | **874,440** |
| Carryover State Appropriation | | 88,360 | **88,360** | | 145,407 | **145,407** | | | **0** |
| New Matching Funds | 357,578 | | **357,578** | 357,578 | | **357,578** | 357,578 | | **357,578** |
| Carryover from Previous Matching | 48,898 | | **48,898** | 80,653 | | **80,653** | | | **0** |
| **Total Revenue** | **406,476** | **905,660** | **1,312,136** | **438,231** | **978,207** | **1,416,438** | **357,578** | **874,440** | **1,232,018** |