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 2005-2006

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Introduction

Consistent with the enabling legislation which led to the formation of the THEC Centers of Excellence in 1984 et seq., the new THEC Center of Excellence for Applied Computational Science and Engineering (CEACSE) has presented a timely opportunity to capitalize on the successful initiative in 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 20 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. The CEACSE officially became enabled on July 1, 2005.

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 or expanded 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 and 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 existing UT SimCenter at Chattanooga with is its general expertise in computational science and applications methodologies that are broadly applicable both in new problem areas and in other disciplines. The SimCenter 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 for instance) 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, through previously obtained funding, has made operational a significant cluster super computer. This machine has a large capacity for performing computational simulation 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

- 121st in the World
- 73rd in the U.S.
- 13th in the South
- 24th among U.S. Universities (*excluding shared resource centers*)
- 6th among U.S. Universities in the South
- 1st among U.S. Universities in the Southeast

* *Based on June 2006* ***TOP500*** *Supercomputer Site Rankings*

Figure 1

To this end there has been a large expansion of the capabilities to expand research and support activities. CEACSE has enabled the expansion of research explorations and activities across the University faculty and SimCenter researchers through its seed funding (Figure 2).

CEACSE Seed Funding Committed for Research Activities

Quantum Measurement and Feedback in Atomic Systems	$18,420
Information Communication Mediator Model in Disaster Management	$33,250
A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysts	$37,870
Geometry Manipulation and Visualization, Computational Simulation and Design	$59,109
Multiprocessor Objective-C computer Systems for High Performance Computing	$61,200
Unstructured Solution Algorithm System Integration, Design and Testing	$66,550
Numerical Solution of the Boltzmann Equation with BGK Approximation	$74,600
Adjoint Method for Magnetohydrodynamic Simulations	$95,391
Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers	$96,255
Development of an Unstructured Grid Algorithm for Turbomachinery	$98,318
Advancement and Verification of the Navier-Stokes Flow Solver for Rocket Motor	$100,078
Computational Engineering with Solid Oxide Fuel Cells	$110,000
Evaluation and Enhancement of an Unstructured Grid Algorithm for Free Surface	$116,160
Computational Analysis and Design of Fuel Cell Components	$124,329
Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing	$148,298
Advanced Turbulence Modeling for Unstructured Topologies	$166,056
Computation of Dynamic Stability and Control Devices	$168,250
Computational Methods for Field Simulations	$168,445

Figure 2

Part of the requirements of the Center is that an external proposal be developed and submitted to a funding agency to continue and expand on the research. Through this first year operation it can be seen (Figure 3) that the activities of the researchers are beginning to bring results. CEACSE has also provided for the inclusion of graduate and undergraduate students.

External Funding Received to Continue the Center's Research Activities

Department of Energy	$579,000
Office of Naval Research	$528,000
Radiance Technologies	$250,000
Science and Technology Applications, LLC	$10,000
Coronal Energy	$192,000
Jackson & Tull/Air Force Research Laboratory*	$190,000
Small Business Administration/The Enterprise Center*	$493,000

*funding pending

Figure 3

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.

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 been successful 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 has provided seed funding for 17 faculty members from various disciplines such as physics, computer science, and computational engineering. One new faculty member has been added to the research program and is

working with seed funding from CEACSE. This particular project appears to be leading to significant external funding. CEACSE seed funding has enabled the support of eight Ph.D graduate students, eleven Masters students, and five undergraduate students. Many of these are still working on seed grants from CEACSE. Indeed, one lecturer in the Computer Science department is working toward a Ph.D. and has received a seed grant. One Ph.D. student working under a seed grant will graduate in December 2006 and has accepted employment as an applications engineer with a computational engineering services company. One Research Associate in Computational Engineering has graduated the Ph.D. program and accepted a faculty research position with the UT SimCenter at Chattanooga and is continuing research on a seed grant. One Ph.D. level graduate student has been fully funded to pursue his research on an externally funded project that resulted from a seed grant. One undergraduate research assistant prepared her Departmental Honors Project based on some of the work that she performed on a CEACSE research grant.

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, where the Center is housed. As an example two companies (Radiance Technologies, Inc. and Adaptive Methods) have opened offices in Chattanooga since these 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 is defining 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 are being investigated. 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 has sought initial and 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 source of continued research funding, e.g. target agency, request for proposal etc. The Center has provided seed funding for initiatives in several of 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.

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 objectives 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 Tennessee.

Research Activities Funded by the Center

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

1. 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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

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.

15. Computational Engineering with Solid Oxide Fuel Cells

- PI: Dr. Jim 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.

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.

17. 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.

18. 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.

Total Seed Funding: $1,742,579

External Funding Received as the Result of the Center's Research Investment

1. Department of Energy (July 2005) ($579,000)
    a. Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III
    b. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams
2. Office of Naval Research (August 2006) ($528,000)
    a. Evaluation and Enhancement of an Unstructured Grid Algorithm for Free Surface; Dr. Robert Wilson

b. Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III
c. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams
d. Development of Parallel Eulerian-Lagrangian Two-Phase Flow Solvers; Dr. Ramesh Pankajakshan
e. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman
f. Development of an Unstructured Grid Algorithm for Turbomachinery; Dr. Kidambi Sreenivas

3. Radiance Technologies (May 2006) (Radiance Technologies (May 2006) ($250,000)
    a. Computational Methods for Field Simulations; Dr. W. Roger Briley
    b. Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams
    c. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman
4. Science and Technology Applications, LLC (August 2006) ($10,000)
    a. Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson, Dr. Steve Karman
5. Coronal Energy (September 2006) ($192,000)
    a. Computational Methods for Field Simulations; Dr. W. Roger Briley

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

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

d. Adjoint Method for Magnetohydrodynamic Simulations; Dr. W. Kyle Anderson, Dr. Steve Karman

6. Jackson & Tull/Air Force Research Laboratory (Pending September 2006) ($190,000)

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

7. Small Business Administration/The Enterprise Center (Pending October 2006) ($493,000)

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

    b. Computational Engineering with Solid Oxide Fuel Cells; Dr. Jim Henry

Total External Funding: $2,242,000

Proposals Submitted for External Funding

1. National Aeronautics and Space Administration

    a. Proposal submitted

    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 submitted

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 submitted

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

   c. 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 submitted

   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 submitted
    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 submitted
    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 submitted and accepted
    b. Title: Unstructured Viscous Free Surface Solver for Predicting Hydrodynamic Performance of High Speed Ships
    c. 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 submitted
    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 submitted

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 submitted

b. Title: Algorithms for Simulation of Electromagnetically Large Structures

c. 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 submitted

b. Title: Analytical Modeling of Liquid Rocket Instability

c. 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 submitted
    b. Title: Computational Analysis of Synthetic Jet Actuators Supporting Aerotonomy, Inc.
    c. Associated CEACSE grants:
        i. Computational Methods for Field Simulations; Dr. W. Roger Briley

13. Coronal Energy, LLC
    a. Proposal submitted
    b. Title: Plasma-Dynamics Software Interface and Test Cases
    c. 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

14. Jackson & Tull/Air Force Research Laboratory
    a. Proposal submitted
    b. Title: Computational Modeling and Simulation Tools for Solid Rocket Motor (SRM) Analysis and Design

c. Associated CEACSE grants:

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

Publications and Presentations of the Center's Research Activities

1. C. Burdyshaw, Achieving Automatic Concurrency Between Field Solver and Adjoint Sensitivity Codes. Ph.D. Dissertation, University of Tennessee at Chattanooga, 2006. *(Extensible Adjoint Methods for Sensitivity Analysis, Error Estimation, and Adaptive Meshing; Dr. W. Kyle Anderson)*
2. D. Ellis, S. Karman, A. Novobilski, R. Haimes, "3D Visualization and Manipulation of Geometry and Surface Meshes," AIAA-2006-0944, 44th AIAA Aerospace Sciences Meeting and Exhibit, Reno, Nevada, Jan. 9-12, 2006. *(Geometry Manipulation and Visualization, Computational Simulation and Design; Ms. Dawn Ellis and Dr. Steve Karman)*
3. K. Sreenivas, L. Taylor, and R. Briley, "A Global Preconditioner for Viscous Flow Simulations at All Mach Numbers," AIAA-2006-3852, 24th AIAA Applied Aerodynamics Conference, San Francisco, California, June 5-8, 2006. *(Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams)*
4. D. Hyams, K. Sreenivas, and D. Whitfield, "Parallel FAS Multigrid for Arbitrary Mach Number, High Reynolds Number Unstructured Flow Solvers," AIAA-2006-2821, 24th AIAA Applied Aerodynamics Conference, San Francisco, California,

June 5-8, 2006. *(Unstructured Solution Algorithm System Integration, Design and Testing; Dr. Daniel Hyams)*

5. N. Alp, F. Jones, R. Bailey, J. Hiestand, "The Use of Taguchi Statistical Methods to Optimize the Design of Biomicroreactors," Institute of Industrial Engineers Annual Conference Proceedings, pp. 108-113, Orlando, Florida, May 2006. *(A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysts; Dr. Frank Jones)*
6. F. Jones, R. Bailey, S. Wilson, J. Hiestand, "The Effects of Engineering Design on Heterogeneous Catalysis in Microchannels," 28th Symposium on Biotechnology for Fuels and Chemicals, Nashville, Tennessee, May 2006, submitted to *Applied Biochemistry and Biotechnology*. *(A Fundamental Study of the Effects of Design on Heterogeneous Biocatalysts; Dr. Frank Jones)*
7. D. S. Nichols III, "Contaminant Transport in an Urban Environment," presented at the East Tennessee Ozone Study 2006 Science Workshop, Oak Ridge, Tennessee, May 2006. *(Advanced Turbulence Modeling for Unstructured Topologies; Dr. D. Stephen Nichols III)*
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Conclusion

CEACSE has established and initiated operation in this the first year. Research funding for a number of diverse projects has begun to engage more faculty and students across the campus. The committed seed funding will enable various faculty to pursue their research, develop opportunities to obtain follow-on support externally in order to expand their efforts and research. 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 as activities accelerate.

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 should assist in increasing the interaction and involvement of students. Additional efforts will need to be defined and initiated increase outreach to pre college students. Additional efforts in this area should be defined. Hopefully this will lead to a stimulated interest in science and engineering.