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Proposal to Establish an Interdisciplinary Program in Computational Science, Mathematics and Engineering (CSME) – Ph.D. Specialization

APPENDICES

PROPOSAL
TO ESTABLISH AN INTERDISCPLINARY GRADUATE PROGRAM IN COMPUTATIONAL SCIENCE, MATHEMATICS AND ENGINEERING (CSME)
PH.D. SPECIALIZATION
May 31, 2006

1.0 INTRODUCTION

1.1 Aims and Objectives

This proposal describes a new interdisciplinary graduate program to be offered at UCSD in Computational Science, Mathematics and Engineering (CSME). Proposed herewith is specialization to existing department-based Ph.D. degree programs resulting in a Ph.D. in (department name) with a specialization in Computational Science. A new stand alone M.S. degree in Computational Science is being proposed under separate cover. Although both Ph.D. and M.S. components of the CSME Program are linked by courses, faculty, space and financial resources, it is our understanding that proposals for new graduate degrees require review by the Systemwide Senate and Office of the President whereas an adjustment to existing Ph.D. programs may be reviewed locally. This proposal, therefore, is a request for local approval of the Ph.D. specialization only.

The CSME Program will draw upon the expertise of faculty from Bioengineering, Biological Sciences, Chemistry and Biochemistry, Computer Science, Electrical and Computer Engineering, Mathematics, Mechanical and Aerospace Engineering, Physics, Structural Engineering, the Scripps Institution of Oceanography as well as research staff with instructional titles from the San Diego Supercomputer Center and the Scripps Research Institute. Computational science refers to the use of computer simulation and visualization for basic scientific research, product development and forecasting. It is an interdisciplinary field that combines mathematics (mathematical modeling, numerical analysis) and computer science (architecture, programming, networks, graphics) with one of the scientific or engineering disciplines. Computational science integrates computer science, the ability to develop mathematical models, the implementation of complex computer algorithms, and the ability to graphically visualize data to provide answers to questions that are difficult or impossible to determine experimentally.

In broad terms, computational science comprises the use of computers to analyze scientific problems. We distinguish it from computer science, which is the study of computers and computation, and from theory and experiment, the traditional forms of science. Computational science seeks to gain understanding principally through the analysis of mathematical models on high performance computers. The term computational scientist has been coined to describe scientists, engineers and mathematicians who apply high performance computer technology in innovative and essential ways to advance the state of knowledge in their respective disciplines. Thus computational science is a blend of applications, computations and mathematics. It is a mode of scientific investigation that supplements the traditional laboratory and theoretical methods of acquiring knowledge. This is done by formulating mathematical models whose solutions are approximated by computer simulations. By making a sequence of adjustments to the model and subsequent computations, one can gain new insights into various areas of science.

This proposal recognizes the nation's growing and continuing need for broadly trained advanced computational scientists in academia, industry and government laboratories. The following remarks of June 17, 2004 by Dr. Arden L. Bement, Jr., Acting Director of the National Science Foundation, express the core importance of the field:

"Computational science is driving discovery and innovation across all fields of science and engineering today. The extraordinary advances in information technology of the past several decades have ushered in a new era of scientific exploration—an era that promises not simply incremental advances, but a revolution in the way we conduct scientific investigation and in the complexity and depth of the new knowledge we can generate."

1.2 Historical Background

Overview: The field of computational science had its beginnings in the early 1940s. With the development of the computer in the midst of World War II, researchers experimented with various problems and methods that could use the advancing computer technology. Numerical tools had existed for centuries, but they were used by hand and were, therefore, slow. The computer motivated mathematicians to reexamine some of the older methods and to develop new ones. Over the years, the increasing speed of computers and advances in numerical methods has made it possible to solve most small problems rapidly, using readily available software. Hence the attention of many computational scientists has turned to the solution of problems so large that they require huge amounts of computer time. This need for vast amounts of computer resources has motivated the development of Computational Science over the last 15 years.

Computational science has emerged as a powerful and indispensable method of analyzing a variety of problems in research, product and process development and manufacturing. Computational simulation is being accepted as a third methodology in scientific research, complementing the traditional approaches of theory and experiment. Computer simulations provide both qualitative and quantitative insights into many phenomena that are too complex to be dealt with by analytical methods or too expensive or dangerous to study by experiments. Many experiments and investigations that have traditionally been performed in a laboratory, a wind tunnel, or the field are being augmented or replaced by computer simulations. Some studies, such as nuclear stockpile integrity and climate change, involve time scales that preclude the use of realistic physical experiments. The availability of high performance computers, graphic workstations, high speed networks, and grids coupled with major advances in algorithms and software, has brought about a revolution in the way scientific and engineering investigations are carried out.

Computational science should not be confused with *computer* science. Computational science focuses on a scientific or engineering problem and draws from computer science and applied mathematics to gain an improved understanding of the problem. Computer science focuses on the computer itself as the focus of research; applied mathematics focuses on the mathematical model as the focus of the research. Even though the areas are quite distinct, many of the topics typically considered to be in the domain of computer science or applied mathematics are of much value in computational science. Traditional or established areas of computational science applications include Computational Fluid Dynamics, Atmospheric Science, Seismology, Structural Analysis, Chemistry, Magnetohydrodynamics, Reservoir Modeling, Global Ocean/Climate Modeling, Environmental Studies, High-density Physics, Nuclear Engineering as well as other areas. Some nontraditional and emerging areas of computational science include Biology, Economics, Finance, Materials Research, Medical Imaging and Animal Science.

Support from the NSF, DOE, and NIH has enabled many of the advances made in computational science research and education. For example, through NSF's Supercomputer Centers Program begun in 1985, five supercomputing centers were established across the country that gained an international reputation for high-performance computing, visualization and desktop software advances. In 1997, the NSF Supercomputer Centers Program was replaced with the NSF Partnerships for Advanced Computational Infrastructure (PACI) program. The National Computational Science Alliance (Alliance) at the University of Illinois - Urbana Champaign and the National Partnership for Advanced Computational Infrastructure (NPACI) at the University of California - San Diego formed the two partnerships in the new PACI program. The Alliance partnership of more than 50 academic partners from across the nation is building a prototype of the country's next-generation information and computational infrastructure, the PACI Grid, to enable scientific discovery and increasingly complex engineering design. The Grid is creating a powerful, seamless and integrated computational problem-solving environment for collaborative, multidisciplinary work on a national scale. In 2000, the NSF awarded the Pittsburgh Supercomputing Center (PSC) a grant to develop a Terascale Computing System (TCS) that will eventually exceed six trillion operations per second (teraflops). NSF has since run several large funding programs in support of computational science research, including the ITR program that currently funds half of UCSD's Center for Theoretical Biological Physics (CTBP).

In addition to providing funding support for basic research in computational science over the last several decades, several years ago, DOE's Office of Science initiated a Computational Science Graduate Fellowship Program in answer to the critical importance of computational science to DOE's core missions and a profound recognition of our nation's growing and continuing need for broadly trained advanced computational scientists in academia, industry and government laboratories. Critically, the Fellowship recognizes that the national academic environment is still working to develop graduate programs with the required mix of skills and knowledge for training leading computational scientists. Focused external support is needed to assist this process. The Fellowship, now jointly funded by the Office of Science and the National Nuclear Security Administration, requires that graduate students plan and follow a course of study that transcends the bounds of traditional academic disciplines. It requires substantive graduate work in each of a scientific or engineering discipline, computer science and applied mathematics. Fellows receive tremendous guidance and support to assist them in becoming scientists and engineers who are able to comfortably communicate across disciplines. Fellows also participate in a 12-week research experience at a DOE lab. In keeping with the DOE CSGF's interdisciplinary emphasis, this practicum must be in an area of research outside of the student's thesis dissertation.

UCSD has strong groups in computational science in many departments including Mathematics, Physics, Chemistry and Biochemistry, Mechanical and Aerospace Engineering, Computer Science and Engineering, Electrical and Computer Engineering, Bioengineering and the Scripps Institution of Oceanography. In addition, UCSD is home to the San Diego Supercomputer Center (SDSC). SDSC staff currently work closely on an immense spectrum of projects, collaborations and codes. Large-scale flagship projects include GEON (geosciences), BIRN and lipid mapping (biosciences), SEEK (ecology), NEES (earthquake engineering), LOOKING (ocean observatories) and others. SDSC hosts the Alliance for Cell Signaling, Biology Workbench, the Protein Data Bank (biosciences), the National Biomedical Computational Resource (NBCR), the National Virtual Observatory data collections (astronomy), and the National Science Digital Library. In addition, SDSC works closely with scientists and engineers on many collaborative projects including Regional Workbench Consortium (for SuperFund), OptIPuter (networking), ROADNet (real-time sensor networks) and TeraGrid (Grid computing).

Biological Sciences: The Division of Biological Sciences has a Computational Neurobiology Graduate Program. It is designed to train young scientists with the broad range of scientific and technical skills that are essential to understand the computational resources of neural systems. This program welcomes students with backgrounds in physics, chemistry, biology, psychology, computer science and mathematics, with courses and research programs that reflect the uniquely computational properties of nervous systems. This interdisciplinary program is closely associated with the Neurosciences Program at UC San Diego and is supported by faculty from several departments and institutions: UC San Diego Division of Biological Sciences, The Salk Institute for Biological Studies, UC San Diego School of Medicine, UC San Diego Institute for Neural Computation, Swartz Center for Computational Neuroscience, the Institute for Nonlinear Science (INLS), and the UC San Diego Departments of Physics, Electrical and Computer Engineering and Cognitive Sciences.

Interactions Between Biological and Physical Sciences: The Center for Theoretical Biological Physics (CTBP) is an interdisciplinary training program funded by a combination of an NSF ITR Award and an NSF Physics Frontier Center Award. This center brings together research faculty, postdoctoral scholars, and graduate students from diverse areas such as mathematics, physics, chemistry and biology to work collaboratively on challenging problems in biophysics and biochemistry. The design of this training program was based in part on the very successful La Jolla Interfaces in Science (LJIS) training program, funded by the Burroughs-Wellcome foundation.

UCSD was recently awarded one of ten new HHMI-NIBIB Interfaces Training Program Awards. This new graduate training program for “Multi-Scale Analysis of Biological Structure and Function” focuses on the education and training of a new generation of biological scientists and engineers at UCSD. The program centers on the development of modern skills in mathematical and computational multi-scale modeling for biological systems.

Chemistry and Biochemistry: The Chemistry and Biochemistry Department at UCSD is heavily involved in computational science research at UCSD. Computational science research activities of the faculty include computer-aided discovery of drugs that bind to RNA targets, computational modeling of temporal correlation in biological signaling pathways, computer modeling and simulation of condensed-phase systems, computational modeling of biomolecular systems, computational analysis of transcription and other biological processes, computer simulations of geophysical and biological processes, Monte Carlo simulations of polymers and microemulsion and computational analysis of condensed phase and biological systems.

Mathematics: The Mathematics Department has been heavily involved in computational science research and education at UCSD for more than three decades. It is the home department of the Computational and Applied Mathematics (CAM) Research Group, consisting of six ladder-rank faculty members in the mathematics department working at the foundations of computational science. Founding members of this group were involved in the LINPACK project and this tradition of cutting edge computational science algorithm and software design and development continues to be a central theme of the group. The CAM group pursues a broad research program in numerical analysis, numerical optimization, numerical ordinary and partial differential equations, approximation theory and applied analysis. Faculty in this group are specialists in adaptive techniques for numerical approximation of partial differential equations, in algorithms for the numerical solution of large-scale optimization and control problems and in supporting areas of mathematics such as abstract approximation theory and partial differential equations. The Mathematics Department also has a substantial number of additional faculty with involvement in other aspects of computational science at varying levels, including research programs on stochastic simulation techniques, applied harmonic analysis and wavelets and computational algorithms for applications in bioinformatics.

Physics: The Physics Department has a sizable group of faculty members whose research is heavily oriented toward the emerging new discipline of computational science. Research topics include computational astrophysics and cosmology studying star formation and the large scale structure of the universe, computational condensed matter physics studying nano-devices, computational quantum field theory studying the four basic forces of nature, computational biological physics of protein folding and other biologically important complex structures, computational nonlinear dynamics, and computational plasma physics. Each faculty member works with graduate students on the listed research topics that will greatly benefit from the new program.

Engineering: The UCSD Jacobs School of Engineering is the youngest and fastest rising among the nation's top 15 engineering schools and the largest engineering school in the University of California system. The Jacobs School research strengths include bioengineering, earthquake and renewal engineering, communications, security and networks, materials, and systems and controls, among others. The Jacobs School B.S., Masters, and Ph.D. programs focus on deep and broad engineering fundamentals in the multi-disciplinary team environment of real-world engineers. The School is home to exciting research facilities, such as the San Diego Supercomputer Center, a national resource for data-intensive computing; the Powell Structural Research Laboratories, the largest and most active in the world for full-scale structural testing; and the California Institute for Telecommunications and Information Technology (CalIT2), which is forging new ground in multi-disciplinary applications for information technology. Among the youngest of the five departments in the Jacobs School, the Bioengineering Department is ranked among the top five graduate programs in the country. Systems biology research programs in the Bioengineering Department cover a wide range of topics, from gene expression analysis to phenotypic functions of microorganisms to integrated functions of whole organs, such as the beating heart.

San Diego Supercomputer Center: The San Diego Supercomputer Center is an organized research unit of UCSD and also a national Data Cyberinfrastructure Center with a mandate to provide services to all domain scientists in this country. The aim of the Center is to provide services and conduct state of the art research in the following areas: 1) Data intensive high end computing, 2) Data management of all kinds ranging from databases to data mining, curation, storage, and archival, 3) Visualization tools and software for scientific research and, finally, 4) Software tools, toolkits, workflows and workbenches for all kinds of domain research. The Center has more than 400 researchers, almost all of them with advanced degrees and most of them with a proven track record of independent research as evidenced by the volume of publications in refereed journals. The Center is well known for its data capabilities and tools like the Storage Resource Broker and ROCKS cluster management software which are world famous. The Center is also well known for its pioneering research in high end computing benchmarking, networking, biology and bioinformatics, ecology and marine sciences and is a world class leader in geosciences and earthquake engineering. The Center supports more than fifty UCSD graduate students who, while anchored in their respective departments with a departmental thesis advisor, do most of their work under supervision of Center personnel. The Center is a unique and valuable resource to the UCSD and UC community in the sense that it combines cutting edge research with running a production facility. The combination ensures that all research conducted in the Center, while state of the art, is firmly grounded in practicality and ensures that the fruits of the research can be implemented in the near future. Given this unique combination of abilities, the Center is well positioned to take a leading role in participating in the proposal to establish a graduate program in computational science.

Scripps Institution of Oceanography: Scripps scientists can be found on every continent and in every ocean as they collaborate on research with colleagues throughout the United States and in 65 nations. Climate change, the loss of biodiversity, rising sea levels, earthquakes, and similar phenomena are among the most critical and complex issues facing society, with computational science providing an important approach to the problems. Computational science related activities at Scripps Institute of Oceanography include the Center for Observations, Modeling and Prediction (COMPAS), formed as a concerted and interdisciplinary effort in numerical modeling and the Scripps Institution of Oceanography Visualization Center which provides a diverse array of research tools for data sharing among distributed locations, live field reports, and real-time data acquisition and presentation.

The Scripps Research Institute: The Scripps Research Institute (TSRI) is one of the country's largest non-profit private research institutes. TSRI is internationally recognized for its research programs in molecular and cellular biology, chemistry, neurosciences, cardiovascular diseases, immunology, and synthetic vaccine development and virology. TSRI is one of the world's leading centers in the study of the basic structure and design of biological molecules. The TSRI campus consists of fourteen laboratory buildings overlooking the Pacific Ocean, and the Institute's staff consists of approximately 270 professors, 800 postdoctoral fellows, 1500 technicians and support staff, and 130 doctoral students. The philosophy of TSRI emphasizes the pursuit of fundamental scientific advances based on a multidisciplinary approach to problem solving, through interdisciplinary collaborations, research, and education programs. Many of the research programs at TSRI involve state-of-the-art computational algorithms and technologies; to support these research programs, the Institute enjoys one of the world's leading private computational capabilities with an array of computers, including a Cray supercomputer.

The Salk Institute: The Crick-Jacobs Center for Theoretical and Computational Biology at the Salk Institute, directed by Terry Sejnowski, has a group of faculty, junior fellows and graduate students who are working on the question of how brains give rise to behavior with a variety of computational and experimental approaches. There are close ties between this Center and the National Center for Microscopy and Imaging Research (NCMIR) and CalIT2 at UCSD.

1.3 Timetable

At the time of this submission, the following are in place.

- Departmental agreements to participate (Appendix A)
- Identification of required and elective courses (Section 5)
- Participating faculty (Section 4.2)
- Governance structure (Sections 1.6, 1.7 and 2.0)

2004-2005	**2005-2006**	**2006-2007**	**2007/2008**
Form faculty committees	Confirm resources	Fall 2006: Begin advertising program	Fall 2007: first students admitted to the program (Existing Ph.D. students may be grandfathered in earlier.)
Develop curriculum	Submit Ph.D. specialization proposal for Campus review and approval Submit M.S. proposal for Systemwide review and approval		
Develop program		Spring 2007: begin accepting applications from interested students	

1.4 Relationship to Existing Programs at UCSD

The Division of Physical Sciences and Jacobs School of Engineering consider Computational Science as a key growth area for UCSD. Several new faculty hires have occurred in the past five years that make this program possible to go forward with now.

1.5 Relationship to Existing Programs at Other Institutions

We know of no approved graduate degree programs in Computational Science in the UC System. However, the UC Davis campus has established a Center for Computational Science and Engineering to support interdisciplinary education in computational science and engineering – both undergraduate and graduate instruction and research. With four existing faculty and plans to recruit five more, formulation and implementation of their academic plan continue, including modeling for a graduate degree program.

Programs outside of the UC system include those at Stanford University, Princeton University, Rice University, the University of Texas at Austin, California Institute of

Technology, the University of Illinois and Purdue University. A brief description of each follows:

Stanford University: Established in 1987, the Scientific Computing and Computational Mathematics (SCCM) Program is a graduate degree awarding program (M.S. and Ph.D.) comprised of faculty from a number of departments. The core courses, which all M.S. and Ph.D. students must complete, are two-year long sequences, one in numerical analysis and the other in methods of mathematical physics. Students must also complete a year of courses in a focused application area, a year of courses in computer science and further courses in applied mathematics and numerical analysis. The choice outside the core sequences is very broad while the core sequences ensure a sound intellectual basis for the program and a commonality among the students.

Princeton University: The Program in Applied and Computational Mathematics (PACM) at Princeton University is an independent academic program leading to the Ph.D. It has its own curriculum, including both courses jointly listed with those offered by participating departments, as well as some courses developed specifically for the graduate program. PACM is not a separate academic department; all participating faculty hold appointments in traditional academic departments on campus. The program is administered by an executive committee consisting of a director and ten committee members. An additional group of some 30 faculty has formal appointments as affiliated faculty in the program. Participating faculty have appointments in the departments of mathematics, physics, chemistry, biology, engineering, computer science, geosciences, economics, atmospheric sciences and ecology giving the program an extremely interdisciplinary character. Doctoral students in the program select their dissertation committee members from among the executive committee and affiliated faculty. The exam structure consists of a first-year exam over course work covering basic techniques in applied and computational mathematics and a second-year exam targeting the student’s research area.

Rice University: The Computational and Applied Mathematics (CAM) Program at Rice University is an independent academic department with graduate programs leading to the Ph.D., M.S. (thesis-based), and M.C.A.M. (course-based master’s) degrees. The program’s 14 participating faculty hold ladder-rank appointments in the CAM department. The CAM program at UT Austin (discussed below), while not an independent academic department, was modeled on the very successful program at Rice.

The University of Texas at Austin: The Computational and Applied Mathematics (CAM) Program at the University of Texas at Austin is an independent academic program leading to the Ph.D. It has its own curriculum, although at present all courses are jointly listed with some offered by participating departments. Fourteen academic departments participate in the program which has an associated ORU.

California Institute of Technology: The Applied and Computational and Mathematics (ACM) Program at the California Institute of Technology is an independent academic department with graduate programs leading to the M.S. and Ph.D. degrees. The 10 participating faculty hold ladder-rank appointments in the ACM department. Doctoral students in the program select their dissertation committee members from among the ACM faculty as well as outside faculty. The exam structure consists of a first-year exam over course work covering basic techniques in applied and computational mathematics and a second-year exam targeting the student's research area.

The University of Illinois: Students participating in the Computational Science and Engineering (CSE) Program become proficient in computing technology, including numerical computation and the practical use of advanced computer architectures as well as in one or more applied disciplines. The program is administered by an Executive Committee composed of one representative from each participating department and chaired by the director. Students must first be admitted to one of the participating departments before enrolling in the CSE option. All CSE courses are cross-listed with one or more of the participating departments. Upon satisfying the degree requirements of both the student's graduate department and the program, the student is awarded a certificate signifying successful completion of a CSE option.

Purdue University: Established in 1995, this program offers specializations at both the M.S. and Ph.D. levels in computational science and computational engineering in 17 departments. The aim of the program is not to produce a student with parts of two degrees but rather a student who has learned how to integrate computing with another scientific or engineering discipline and who is able to make original contributions in both disciplines.

1.6 Program Administration

The Mathematics Department will serve as the administrative home for the proposed program. This organizational plan will leverage existing strengths that, along with a small additional investment in staff, will provide an efficient management core. Moreover, the historical and continuing strengths of the Mathematics Department in the core foundational areas of computational science such as numerical analysis and partial differential equations makes the Mathematics Department a natural foundation for the program.

The CSME graduate program will be managed principally by an executive committee of 10-15 participating faculty, together with a director (or co-directors), to be selected initially by the Division of Physical Sciences. To ensure that the program remains interdisciplinary, dynamic, and representative of the wide range of interests of the faculty at UCSD, co-directors will always be selected from different academic departments, and the executive committee will strive to have at least one representative faculty from each of the participating departments.

The director(s) will work with the executive committee, an admissions committee and qualifying exam committee in the management of the program. The executive committee will have general oversight of the program with particular emphasis on participation in management decisions, program evaluation and curricular functions.

CSME Program Directors

Name	Degree	Department	Division
Holst, Michael	Ph.D.	Mathematics	Physical Sciences
Kuti, Julius	Ph.D.	Physics	Physical Sciences

CSME Program Executive Committee

Name	Degree	Department	Division
Baden, Scott	Ph.D.	CSE	JSOE
Bank, Randolph	Ph.D.	Mathematics	Physical Sciences
Berman, Frances	Ph.D.	CSE/SDSC	JSOE
Bewley, Thomas	Ph.D.	MAE	JSOE
Holst, Michael	Ph.D.	Mathematics	Physical Sciences
Krysl, Petr	Ph.D.	Structural Engineering	JSOE
Kuti, Julius	Ph.D.	Physics	Physical Sciences
McCammon, Andrew	Ph.D.	Chemistry & Biochemistry	Physical Sciences
McCulloch, Andrew	Ph.D.	Bioengineering	JSOE
Norman, Michael	Ph.D.	Physics	Physical Sciences
Orcutt, John	Ph.D.	IGPP	SIO
Pozrikidis, Constantine	Ph.D.	MAE	JSOE
Remmel, Jeffrey	Ph.D.	Mathematics	Physical Sciences
Sejnowski, Terrence	Ph.D.	Biological Sciences	Biological Sciences

CSME Program Participating Faculty
See “Affiliated Faculty” in Section 4.2 below.

Admissions Committee
Each year the Executive Committee will choose a faculty member from each participating department to serve on the Admissions Committee for the graduate program. The executive committee will ensure that this service work is shared equally among the participating faculty. Since admission into the graduate program requires simultaneous admission into the home department, it is understood that the assigned faculty member will need to work closely with the admissions committee in the home department. The CSME Admissions Committee will meet at the appropriate time each year to evaluate and rank the pool of applicants for admission into the program.

Qualifying Exam Committee
Each year the Executive Committee will choose a faculty member from each participating department to serve on the Qualifying Exam committee for the specialization. The executive committee will ensure that this service work is shared equally among the participating faculty. The Qualifying Exam committee will meet regularly to discuss issues that arise with the three quarter-length qualifying exam courses and their corresponding final exams which together serve as the qualifying examination for the specialization. The committee will also be responsible for hearing and deciding on any petitions for exceptions to the qualifying exam policies described in this document.

Doctoral Committee
Constitution of the doctoral committee will be enforced in accordance with University and home department regulations with a minimum of five faculty members consisting of three from the home department and two from outside the department. The Chair will be a member of the home department who is also affiliated with the CSME Program.

1.7 Plan for Evaluation

In keeping with established campus procedures, we plan an internal review by the Executive Committee, the campus Graduate Council and the Office of Graduate Studies and Research approximately eight years after admitting the first class of students.

2.0 PROGRAM

2.1 Overview

The Ph.D. specialization in Computational Science at UCSD will leverage the strength of the existing mathematics, science, and engineering departments by being home-department based rather than a stand-alone program. To accomplish this, the proposed structure of the Ph.D. specialization is that each participating department will have a Ph.D. degree with a new specialization, Computational Science. For example, a physics student would obtain a Ph.D. with a specialization in Physics/Computational Science, a mathematics student would obtain a Ph.D. with a specialization in Mathematics/Computational Science, an engineering student would obtain a Ph.D. with a specialization in Engineering/Computational Science and so forth. The best computational scientists are those with a solid background in their respective fields and, therefore, the structure of the program is designed to take advantage of the outstanding basic training that the participating departments already provide in their respective areas. Each student will be expected to pass qualifying exams in their home department that will be adapted in some way by the individual departments to allow the students to take part in the CSME graduate program. In addition, there will be a common qualifying exam that all Ph.D. students in CSME must pass. Details about the structure of the qualifying exams will be given below.

As a result of this structure, we believe that the students we train will be well-prepared for faculty positions in traditional departments in their respective fields in addition to being prepared for positions in future computational science departments. Moreover, we believe the proposed program will place UCSD at the forefront of modern training programs in Computational Science.

The new courses developed in support of the Ph.D. specialization (see below for course descriptions) will join our existing courses in computational science as general service courses that will benefit the entire UCSD campus as well as local industry in the San Diego area. The courses will also be a resource for graduate students in engineering and the sciences who do not necessarily want to focus on computational science, but, nevertheless, have need for some simulation or large computation in their research. Such students can use the core courses to gain a solid introduction to such topics as algorithms, parallel computing or stochastic methods that they may need to understand to further their research. Thus we expect that the courses that we will develop for the CSME Program will be of use to many graduate students in engineering and science.

2.2 Undergraduate Preparation

No requirements will be imposed beyond those of the admitting home department.

2.3 Foreign Language

No requirements will be imposed beyond those of the admitting home department.

2.4 Program of Study

The proposed CSME Program at UCSD consists of both a 4-5 year home department-based Ph.D. specialization and a stand-alone 2-year M.S. program. The structure of the Ph.D. component is described below.

Ph.D. Specialization Structure

The Ph.D. component is designed to allow a student to obtain standard basic training in their chosen field of science, mathematics or engineering with training in computational science integrated into their graduate studies. Requirements consist of the home department requirements and proficiency, qualifying and elective course requirements as outlined below.

> *Proficiency Requirements:* Substantial background in computing is now part of any undergraduate program in science and engineering. Success in the proposed graduate program relies on these skills. Therefore, Ph.D. students must demonstrate advanced undergraduate-level proficiency in numerical analysis and in computer algorithms and data structures. Proficiency may be demonstrated by taking UCSD's courses in both subjects while enrolled in the graduate program (4 units per course):
>
> (1) Numerical Methods (MATH 174/274 or MAE 290A)
> (2) Data Structures and Algorithms (CSE 100/101)
>
> Alternatively, proficiency in the material contained in these courses may be satisfied by having previously taking these or equivalent courses at other institutions, or through other evidence of sufficient knowledge of this material. Demonstrating proficiency without taking these courses at UCSD is subject to approval by the Executive Committee on an individual basis.
>
> *Qualifying Requirements:* In addition to the home department qualifying exam requirements, Ph.D. students must pass the final exams in three qualifying exam courses. It is expected that most students will register for and take these courses (4 units per course), but the Executive Committee may allow an exceptionally well-prepared student to take the final exams without taking the courses. The three qualifying exam courses have been selected to provide a general broad set of tools in computational science and are as follows:
>
> (1) MATH 275 or MAE 290B (Numerical PDEs)
> (2) PHYS 244 or CSE 260 (Parallel Computing)
> (3) Course to be selected from LIST A
>
> LIST A: CSME Qualifying Exam Courses. Courses taken to satisfy the qualifying requirements can not count toward the elective requirements.
>
> (1) PHYS 243 (Stochastic Methods)
> (2) MATH 270A, B or C (Numerical Analysis; Not permitted for Math Students)
> (3) MATH 272 A, B or C (Advanced Numerical PDEs)
> (4) MAE 223 (Computational Fluid Dynamics)

(5) MAE 232 A or B (Computational Solid Mechanics)
(6) MAE 280 A or B (Linear Systems Theory)
(7) (To be determined by Executive Committee)

Elective Requirements: To encourage Ph.D. students to both broaden themselves in an area of science or engineering as well as to obtain more specialized training in specific areas of computational science, students will be required to take and pass three elective courses from the following approved list (4 units per course). The Executive Committee may approve the use of courses not appearing on the following list on a case-by-case basis. Courses taken to satisfy the elective requirements can not count toward the qualifying requirements.

LIST B: Relevant Elective Graduate Courses in Mathematics, Science, and Engineering
(1) MATH 270ABC (Numerical Analysis; Not permitted for Math students)
(2) MATH 271ABC (Optimization)
(3) MATH 272ABC (Advanced Numerical PDEs)
(4) MATH 273ABC (Computational Mathematics Project)
(5) PHYS 141/241 (Computational Physics I)
(6) PHYS 142/242 (Computational Physics II)
(7) PHYS 221 AB (Nonlinear dynamics)
(8) CHEM 215 (Modeling Biological Macromolecules
(9) BGGN 260 (Neurodynamics)
(10) (To Be Determined by Executive Committee)

Program Policies: The following is a list of policies for the Ph.D. Specialization with regard to Proficiency, Qualifying, and Elective Requirements:

(1) Proficiency must be satisfied by the end of the first year.
(2) The Qualifying Exams must be passed by the end of the second year or, on petition, by end of the third year.
(3) The qualifying exams can be attempted repeatedly but no more than once per quarter per subject.
(4) The qualifying exams in the home department and the CSME qualifying exams must all be passed before the student is permitted to take the candidacy (senate) exam.
(5) Two electives outside the home department must be taken.
(6) The two electives can be taken at any time before defending the thesis.
(7) One of the electives may be taken Pass/Fail; the other must be taken for a letter grade.
(8) Existing Ph.D. students in home departments may elect to participate in the CSME Program the first year it is online, subject to approval of the Executive Committee.

2.5 Field Examinations

No requirements will be imposed beyond those of the admitting home department.

2.6 Qualifying Examinations

Ph.D. students must pass the qualifying examination according to the timetables specified above. The exams consist of the final exam for the particular qualifying course. Satisfying the qualifying exam requirements consists of passing all three qualifying exams.

2.7 Thesis/Dissertation

Ph.D. students must complete a dissertation which meets all requirements of the home department. In addition, it is expected that the Ph.D. dissertation will be interdisciplinary in nature and involve some aspect of computational science.

2.8 Final Examination

Ph.D. students must meet the final examination requirements of the home department.

2.9 Explanation of Special Requirements

The Ph.D. specialization requires that the student complete all home department requirements for the Ph.D. along with satisfying the CSME qualifying requirements.

2.10 Relationship of M.S. and Ph.D. Programs

The Ph.D. component is based in home participating departments whereas the M.S. component is a stand-alone program. However, the two components share the CSME qualifying exam courses, along with elective courses in computational science.

We expect that some students from the M.S. will decide to continue their education and get a Ph.D. with a specialization in Computational Science. Such a student would have to apply to one of the participating departments, be admitted to that department's graduate program, and then be admitted by the CSME program like any other student who wants to be part of the CSME program. It is also possible that some students who decide to not complete their Ph.D. may want to transfer to the M.S. program. We expect that this will be rare since such students can just get a Master's degree in their home department. Nevertheless, it seems reasonable to allow such transfer to the M.S. program. However, since the M.S. program is a stand alone program, the student would have to apply and be admitted to the M.S. program to make such a transfer.

2.11 Special Preparation for Careers in Teaching

The Ph.D. specialization does not contain special provisions beyond those of the home department. Appropriate teaching preparation varies greatly among fields in science, mathematics, and engineering and this should be left to the home department.

2.12 Time Limits

Normative Time to Degree: Ph.D. students must complete their home department degree requirements as well as the CSME qualifying exams. However, on an individual basis, participating departments may alter their qualifying requirements to allow the students to meet the CSME qualifying requirements without adding substantial time to degree. Therefore, it is expected that the normal time to degree will be 5 years.

Other Time Limits: Ph.D. students will be subject to all time limits of the home department.

3.0 PROJECTED NEED

3.1 Student Demand

We anticipate that each department will admit 3-5 students into their departments for participation in the Ph.D. component of CSME Graduate Program, leading to a steady state of 12-15 students within each department participating in the Program at any particular time. Individual departments may decide to decrease or increase the number of students participating in the program based on funding support, need, and other considerations, however, the projected total steady-state enrollment for the Ph.D. specialization is 32-40 students. We anticipate 30-35 M.S. students at steady state.

3.2 Opportunities for Placement of Graduates

The need for well-trained scientists and engineers with specialized skills in computational science in industry, national laboratories, and academic institutions is well-established. We believe that both Ph.D. and M.S. graduates from the CSME will be well-positioned to compete effectively for the best jobs in these areas. Historically, simulation has been used as a qualitative guide for design and control, but has often not been expected to provide accurate results for realistic physical systems. Increasingly, simulation is being used in a more quantitative way as an integral part of the manufacturing, design and decision-making processes and as a fundamental tool for scientific research. Below we list a few areas in science and industry where computational science has played, and is expected to continue to play, a pivotal role and for which graduates of our program will be well-equipped to work in.

Computational mechanics. Computational mechanics is an integral and major subject of research in many fields of science and engineering, design and manufacturing. Major established industries such as the automobile, aerospace, atmospheric sciences, chemical, pharmaceutical, petroleum, electronics and communications as well as emerging industries such as biotechnology, nanotechnology and information technology rely on computational mechanics-based capabilities to model and numerically simulate complex systems for the analysis, design, and manufacturing of high-technology products. Rapid advances in computer architecture, hardware, software technology and tools, and numerical and non-numerical algorithms are making significant contributions to the development of computational models and methods to model materials and analyze and design complex engineering systems.

Biological and Medical Sciences. Computational science is rapidly becoming indispensable to the biological and medical sciences. Simulation plays a major role in the conceptual development of medical devices, both those used in diagnostic procedures (electromagnetic, ultrasonic, etc.) and in design of artificial organs (hearts, kidneys, etc.). Biomedical optics depends heavily on computational modeling in uses in detection and treatment in oncology, ophthalmology, cardiology and physiology. Computational modeling plays a fundamental role in the emerging efforts to combine mathematics and biology in the genomic sciences (genome sequencing, gene expression profiling, genotyping, etc.) In this area one needs large scale simulations with complex computational models to develop new theoretical/conceptual models and understanding of molecular level interactions.

Chemistry. Computational chemistry is widely used in academic and industrial research. Computed molecular structures, for example, are very often more reliable than experimentally determined ones. According to “Chemical & Engineering News,” computational chemistry has developed from a “nice to have” to a “must-have” tool. The main incentive of computational chemistry is the prediction of chemical phenomena based on models which relate either to first principles theory (“rigorous models”), to statistical ensembles governed by the laws of classical physics or thermodynamics or simply to empirical knowledge. In real problem solving situations, these models are often combined to form “hybrid models” where only the critical part of the problem is treated at the rigorous level of theory. Rigorous theory in the molecular context is synonymous with quantum mechanics, i.e., solving the Schrödinger equation for a molecular complex with or without the presence of external perturbation (photons, electric fields, etc.) There are a number of methods available which provide approximate solutions to the Schrödinger equation, Hartree-Fock and Density Functional theory, for example. Simulation is used to predict properties of large and complex entities such as a liquid, the folding of a protein in solution or the elasticity of a polymer. Finally, empirical models most often try to establish correlations between the structure of a molecule and its (pharmaceutical) activity. Simulations and quantum chemical calculations, on the other hand, are very often extremely compute-intensive due to the number of degrees of freedom and the complexity of the terms to be evaluated. The high accuracy required in these calculations sets restrictions with regard to the method used to solve the partial differential equations (PDEs) involved.

Materials. The challenge in materials research is to invent new materials and to perfect existing ones by fabrication and processing so that they have the desired performance and environmental response. For example, there are many new and important applications for thin films including silicon-based microelectronics, compound semiconductors, opto-electronics devices, high-temperature superconductors and photovoltaic systems. The growth of such thin films, which can be accomplished via processes such as chemical vapor deposition (CVD), is sensitive to many factors in the manufacturing process. Simulation is an essential tool for understanding this process, and requires the development of mathematical models and computational techniques. Process control, which is an order of magnitude more computationally complex than simulation, is emerging as an essential tool in fabrication. Recently, large scale complex computational modeling has been used to design high pressure, high throughput CVD reactors to be used as enabling devices in the production of new and exotic materials.

Bioengineering. Historically, engineers have used chemistry, thermodynamics and transport to design chemical processes. Now these fundamental processes are applied to the understanding of complex biological phenomena that are governed by the same physical laws. Computer models are being used to understand and to develop treatments for glaucoma, to understand and to fabricate bioartificial materials (for example, bioartificial arteries) and for studying the normal and pathologic response of soft hydrated tissues in the human musculoskeletal system.

Weather and climate prediction. Future energy and environmental strategies will require unprecedented accuracy and resolution for understanding how global changes are related to events on regional scales where the impact on people and the environment is the greatest. Achieving such accuracy means bringing the resolution used in weather forecasting to the global predictions. This is not practical currently because of the very large amounts of data storage and long computation times that are required. A major advance in computing power will enable scientists to incorporate knowledge about the interactions between the oceans, the atmosphere and living ecosystems such as swamps, forests, grasslands and the tundra into the models used to predict long-term change. Climate modeling at the global, regional and local levels can reduce uncertainties regarding long term climate change, provide input for the formulation of energy and environmental policy, and abate the impact of violent storms.

Combustion. Accurate simulation of combustion systems offers the promise of developing the understanding needed to improve efficiency and reduce emissions as mandated by U. S. public policy. Combustion of fossil fuels accounts for 85% of the energy consumed annually in the U. S. and will continue to do so for the foreseeable future. Achieving predictive simulation of combustion processes will require terascale computing and an unprecedented level of integration among disciplines including physics, chemistry, engineering, mathematics and computer science.

Nuclear stockpile stewardship. While new weapon production has ceased, the ability to design nuclear weapons, analyze their performance, predict their safety and reliability and certify their functionality as they age is essential for conscientious management of the enduring U. S. nuclear stockpile. Dramatic advances in computer technology have made virtual testing and prototyping viable alternatives to traditional nuclear and non-nuclear test-based methods for stockpile stewardship. Rudimentary versions of virtual testing and prototyping exist today. To meet the needs of stockpile stewardship for the near future, however, requires high-performance computing far beyond our current level of performance. The ability to estimate and manage uncertainty in models and computations is critical for this application and increasingly important for many others.

Simulation, design and control of vehicles. It is now standard practice in the design of mechanical systems such as vehicles, machines or robots to use computer simulation to observe the dynamic response of the system being designed. Computer-aided design drastically reduces the need to construct and test prototypes. Simulation is used not only to improve performance, but also for safety and ergonomics. Real-time simulation with operator in the loop and/or hardware in the loop presents substantial challenges for algorithms and software.

Aircraft design. Since the early days of computing, computational simulation has been used in the performance analysis and design of aircraft components such as the analysis of lift and drag of airfoil designs. As computations become more sophisticated and computers more powerful, computational simulation is used as an essential tool in the complete design process. For example, the Boeing 777 was the first jetliner to be 100% digitally designed using 3D solid modeling. Throughout the design process, the airplane was preassembled on the computer, eliminating the need for a costly full-scale mark-up. Computational science will play an increasingly important role in the entire design and analysis process as capabilities improve for such things as numerical modeling of combustion for engine design.

3.3 Importance to Discipline

This proposal has arisen to address the needs of a broad spectrum of research faculty across the UCSD campus. It was recognized that a new type of training was required to address the growing demand for specialized skills in computational science and that the most effective means to address this issue was to bring together the best ideas, courses and faculty to collectively build a strong interdisciplinary training program in Computational Science, Mathematics and Engineering at UCSD.

3.4 Needs of Society

As remarked in the introduction to this proposal, Computational Science is a newly emerging scientific discipline that uses tools from computer science and applied mathematics to study problems in science whose solutions require extensive computation. This proposal recognizes the nation's growing and continuing need for broadly trained advanced computational scientists in academia, industry and government laboratories. The remarks of June 17, 2004 by Dr. Arden L. Bement, Jr., Acting Director of the National Science Foundation, were mentioned in the introduction to this proposal. We point out also that the President's Information Technology Advisory Committee (PITAC) gave a report to the President in June 2005 entitled *"Computational Science: Ensuring America's Competitiveness."* In the cover letter to their report, the committee states that *"Computational science is one of the most important technical fields of the 21st century because it is essential to advances throughout society."*

3.5 Relationship of the Program to Research and/or Professional Faculty Interests

The program envisioned here has been produced after months of extensive discussion among most of the computational scientists at UCSD in the Departments of Mathematics, Physics, Chemistry and Biochemistry, Biology, Mechanical and Aerospace Engineering, Structural Engineering, Bioengineering, Electrical and Computer Engineering, Computer Science and Engineering, the San Diego Supercomputer Center and the Scripps Institution of Oceanography. The result is a graduate program that addresses the need for the development of core mathematical and computer science research tools along with the opportunity for advanced training and specialization in most of the disciplines at UCSD that benefit from modern computational science techniques. The graduate program was designed by some of the most active research faculty on campus and, as a result, recognizes the importance of flexibility to address the specific needs of research faculty as well as those of the student.

3.6 Program Differentiation

UCSD is exceptionally positioned to provide a premier graduate program in Computational Science, Mathematics and Engineering. The uniform strength of the existing graduate programs in science, mathematics, and engineering provides an outstanding base of operations for the program described here. Moreover, UCSD has a tradition of research collaboration across science departments that is unique, in many respects, to UCSD such as the Center for Theoretical Biological Physics (CTBP), the Institute for Nonlinear Science (INLS), the La Jolla Interface in Science Program (LJIS) and many others over the years. The proposed graduate program continues this tradition of interdisciplinary research and education. The strength of the participating mathematics, science, and engineering departments combined with the truly interdisciplinary nature of research at UCSD creates an institutional setting for the proposed graduate program that we feel is unmatched anywhere else in the country.

4.0 FACULTY

4.1 Critical Mass of Faculty to Serve Program

We currently have the critical mass of faculty necessary to serve this program.

4.2 Affiliated Faculty

CSME Program Affiliated Faculty

Name	Degree	Rank	Department	Division
Abarbanel, Henry	Ph.D.	Professor	Physics	Physical Sciences/SIO
Baden, Scott	Ph.D.	Professor	CSE	JSOE
Bank, Randolph	Ph.D.	Professor	Mathematics	Physical Sciences
Benson, David	Ph.D.	Professor	MAE	JSOE
Berman, Frances	Ph.D.	Professor/Director	CSE/SDSC	JSOE
Bewley, Thomas	Ph.D.	Associate Professor	MAE	JSOE
Bunch, James	Ph.D.	Professor	Mathematics	Physical Sciences
Buss, Samuel	Ph.D.	Professor	Mathematics	Physical Sciences
Cheng, Li Tien	Ph.D.	Associate Professor	Mathematics	Physical Sciences
DiVentra, Massimilliano	Ph.D.	Associate Professor	Physics	Physical Sciences
Gill, Phillip	Ph.D.	Professor	Mathematics	Physical Sciences
Holst, Michael	Ph.D.	Professor	Mathematics	Physical Sciences
Krysl, Petr	Ph.D.	Associate Professor	SE	JSOE
Kuti, Julius	Ph.D.	Professor	Physics	Physical Sciences
Li, Bo	Ph.D.	Associate Professor	Mathematics	Physical Sciences
McCammon, Andrew	Ph.D.	Professor	Chemistry/Biochemistry	Physical Sciences
McCulloch, Andrew	Ph.D.	Professor	Bioengineering	JSOE
Nomura, Keiko	Ph.D.	Associate Professor	MAE	JSOE
Norman, Michael	Ph.D.	Professor	Physics	Physical Sciences
Orcutt, John	Ph.D.	Professor	IGPP	SIO
Padoan, Paolo	Ph.D.	Assistant Professor	Physics	Physical Sciences
Palsson, Bernard	Ph.D.	Professor	Bioengineering	JSOE
Paturi, Ramamohan	Ph.D.	Professor	CSE	JSOE
Pozrikidis, Constantine	Ph.D.	Professor	MAE	JSOE
Quest, Kevin	Ph.D.	Professor	ECE	JSOE
Remmel, Jeffrey	Ph.D.	Professor	Mathematics	Physical Sciences
Sarkar, Sutanu	Ph.D.	Professor	MAE	JSOE
Sejnowski, Terrence	Ph.D.	Professor	Biological Sciences	Biological Sciences
Tesler, Glenn	Ph.D.	Assistant Professor	Mathematics	Physical Sciences
Wang, Wei	Ph.D.	Assistant Professor	Chemistry/Biochemistry	Physical Sciences
Wuerthwein, Frank	Ph.D.	Associate Professor	Physics	Physical Sciences

4.3 Faculty CV (See Appendix B)

4.4 Letters of Support – Participating Departments (See Appendix A)

5.0 COURSES

5.1 Existing Courses

Bioengineering:

BENG 184/BIMM 184/CSE 184/CHEM 184. Computational Molecular Biology (4) (Cross-listed as BIMM 184, CSE 184, and Chem. 184.) This advanced course covers the application of machine learning and modeling techniques to biological systems. Topics include gene structure, recognition of DNA and protein sequence patterns, classification, and protein structure prediction. Pattern discovery, hidden Markov models/support vector machines/neural network/profiles, protein structure prediction, functional characterization of proteins, functional genomics/proteomics, metabolic pathways/gene networks. *Prerequisites: BENG 181 or BIMM 181 or CSE 181; BENG 182 or BIMM 182 or CSE 182 or CHEM 182; Bioinformatics majors only. (W)*

BENG 213. Systems Biology and Bioengineering III: Building and Simulating Large-scale In Silico Models (4) Mathematical models of reconstructed reaction networks and simulation of their emergent properties. Classical kinetic theory, stochastic simulation methods and constraints-based models. Methods that are scalable and integrate multiple cellular processes will be emphasized. Existing genome-scale models will be described and computations performed. Emphasis will be on studying the genotype-phenotype relationship in an in silico model driven fashion. Comparisons with phenotypic data will be emphasized. *Prerequisite: BENG 212 or consent of instructor. (S)*

BENG 247C. Bionanotechnology (4) Topics include: nanosensors and nanodevices for both clinical diagnostics and biowarfare (bioterror) agent adetection; nanostructures for drug delivery; nanoarrays and nanodevices; use of nanoanalytical devices and systems; methods and techniques for modification or functionalization of nanoparticles and nanostructures with biological molecules; nanostructural aspects of fuel cells and biofuel cells; potential use of DNA and other biomolecules for computing and ultra-high-density data storage. *Prerequisite: graduate standing. (S)*

BENG 275. Computational Biomechanics (4) Finite element methods for anatomical modeling and boundary value problems in the biomechanics of tissues and biomedical devices. Nonlinear biodynamics, heat flow, cardiac impulse propagation, anatomic modeling, and biomechanics. *Prerequisite: consent of instructor. (*F)

Biological Sciences:

BIPN 146. Computational Neurobiology (4)
An exploration of computational brain models, including biophysical models of single neurons, small neural circuits, and larger scale network models. *Prerequisites: BILD 12 or BIPN 140 or Psych. 106 or Cog Sci. 107 recommended.*

BGGN 260. Neurodynamics (4)
Introduction to the nonlinear dynamics of neurons and simple neural systems through nonlinear dynamics, bifurcation theory and chaotic motions. The dynamics of single cells is considered at different levels of abstraction, e.g., biophysical and “reduced” models for analysis of regularly spiking and bursting cells, their dynamical properties and their representation in phase space.

Chemical Engineering:

CENG 100. Process Modeling and Computation in Chemical Engineering (4)
Introduction to elementary numerical methods with applications to chemical engineering problems using a variety of problem solving strategies. Error analysis. Concepts of mathematical modeling, material and energy balances and probability and statistics with applications to design problems. *Prerequisites: admission to the chemical engineering or bioengineering major only and grades of C\u2013 or better in MAE 9 or 10, and Chem. 6C.*

Chemistry:

CHEM 215. Modeling Biological Macromolecules (4)
Use of computer graphics and modeling methods in the study of biological macromolecules. The course will cover basic methods and techniques. The objective is to provide a good working knowledge of the critical features of the methods and to provide a foundation for further study for those who wish to pursue these methods as research topics. Chem. 215 students will be required to complete additional coursework beyond that expected of students in Chem. 115. *Prerequisite: Chem. 114A or equivalent.* (May not be offered every year.)

CHEM 285. Introduction to Computational Chemistry (4)
Course in computational methods building on a background in mathematics and physical chemistry. Brief introduction and background in computational theory, molecular mechanics, semi-empirical methods, and ab initio-based methods of increasing elaboration. Emphasis on applications and reliability. Chem. 285 students will be required to complete additional coursework beyond that expected of students in Chem. 185. *Prerequisites: Chem. 126 or 133 and Math. 20C.* (May not be offered every year.)

Computer Science and Engineering:

CSE 100. Advanced Data Structures (4) Descriptive and analytical presentation of data structures and algorithms. Lists, tables, priority queues, disjoint subsets, and dictionaries data types. Data structuring techniques include linked lists, arrays, hashing, and trees. Performance evaluation involving worst case, average and expected case, and amortized analysis. Credit not offered for both Math. 176 and CSE 100. Equivalent to Math. 176. *Prerequisites: CSE 12, CSE 21 or Math. 15B, and CSE 30, or consent of the instructor. Majors only.*

CSE 101. Design and Analysis of Algorithms (4) Design and analysis of efficient algorithms with emphasis of non-numerical algorithms such as sorting, searching, pattern matching, and graph and network algorithms. Measuring complexity of algorithms, time and storage. NP-complete problems. Credit not offered for both Math. 188 and CSE 101. Equivalent to Math 188. Prerequisites: CSE 12, CSE 21 or Math. 15B or Math. 100A or Math. 103A and CSE 100 or Math. 176. Majors only.

CSE 260. Parallel Computation (4) Overview of parallel hardware, algorithms, models and software. Topics include Flynn's taxonomy, interconnection networks, memory organization, a survey of commercially available multiprocessors, parallel algorithm paradigms and complexity criteria, parallel programming environments and tools for parallel debugging, language specification, mapping, performance, etc.

Electrical and Computer Engineering:

ECE 240B. Optical Information Processing (4) Space-bandwidth product, superresolution, space-variant optical system, partial coherence, image processing with coherent and incoherent light, processing with feedback, real-time light modulators for hybrid processing, nonlinear processing. Optical computing and other applications. *Prerequisite: ECE 182 or equivalent. (W)*

ECE 241B. Optical Devices for Computing. (4) Application of electro-optic, magneto-optic, acousto-optic, and electro-absorption effects to the design of photonic devices with emphasis on spatial light modulation and optical storage techniques. *Prerequisites: ECE 240A, C, or consent of instructor. (F)*

ECE 241BL. Optical Signal Processing Laboratory (2) Construction and characterization of Fourier/Fresnel transform, coherent/incoherent, imaging-processing systems. Design, coding, fabrication of spatial filters, computer-generated holograms. Experiments in nonlinear photorefractive phenomena and image-processing applications. Construction of vector-matrix multipliers. Optical systems design using Code-V. *Prerequisites: ECE 181, 182, 183, or consent of instructor. (This course is cojoint with ECE 185. Graduate stduents will choose 50 percent of the experiments and receive two units of credit.) (W)*

ECE 47C. BioNanotechnology (4) Topics include: nanosensors and nanodevices for both clinical diagnostics and biowarfare (bioterror) agent detection; nanostructures for drug delivery; nanoarrays and nanodevices; use of nanoanalytical devices and systems; methods and techniques for modification or functionalization of nanoparticles and nanostructures with biological molecules; nanostructural aspects of fuel cells and bio-fuel cells; potential use of DNA and other biomolecules for computing and ultra-high-density data storage. Cross-listed with BENG 247C. *Prerequisite: graduate standing. (S)*

ECE 270A-B-C. Neurocomputing (4-4-4) Neurocomputing is the study of biological information processing from an artificial intelligence engineering perspective. This three-quarter sequence covers neural network structures for arbitrary object (perceptual, motor, thought process, abstraction, etc.) representation, learning of pairwise object attribute descriptor antecedent support relationships, the general mechanism of thought, and situationally responsive generation of movements and thoughts. Experimental homework assignments strongly reinforce the fundamental concepts and provide experience with myriad associated technical issues. *Prerequisite: graduate standing, an understanding of mathematics through basic linear algebra and probability, or consent of instructor. (F,W,S)*

ECE 275A. Parameter Estimation I (4) Linear last squares (batch, recursive, total, sparse, psuedoinverse, QR, SVD); statistical figures of merit (bias, consistency, Cramer-Rao lower-bound, efficiency); maximum likelihood estimation (MLE); sufficient statistics; algorithms for computing the MLE including the expectation maximation (EM) algorithm. The problem of missing information; the problem of outliers. *Prerequisites: ECE 109 and ECE 153 with grades of C\u2013 or better. (F)*

ECE 291. Industry Sponsored Engineering Design Project (4) One or two students as a group design, build, and demonstrate an engineering project that is sponsored by local industry. All students give a weekly progress report on their tasks and write a final report. The projects originate from the actual needs of industry in the general area of electrical and computer engineering. This course may count towards the fulfillment of the MEng degree. Individual final exam and final presentation. *Prerequisite: ECE 230 or 240 or 251 or 253 or 258 or equivalent.*

Mathematics:

MATH 170A Numerical Linear Algebra (4)
Analysis of numerical methods for linear algebraic systems and least squares problems. Orthogonalization methods. Ill conditioned problems. Eigenvalue and singular value computations. Three lectures, one recitation. *Prerequisites: Math. 20F and knowledge of programming. (F,S)*

MATH 170B Numerical Analysis (4)
Rounding and discretization errors. Calculation of roots of polynomials and nonlinear equations. Interpolation. Approximation of functions. Three lectures, one recitation. *Prerequisites: Math. 20F and knowledge of programming.* (W)

MATH 170C Numerical Ordinary Differential Equations (4)
Numerical differentiation and integration. Ordinary differential equations and their numerical solution. Basic existence and stability theory. Difference equations. Boundary value problems. Three lectures, one recitation. Math. 170B or consent of instructor. (S) *Prerequisites: None*

MATH 171A-B Mathematical Programming-Numerical Optimization (4-4)
Mathematical optimization and applications. Linear programming, the simplex method, duality. Nonlinear programming, Kuhn-Tucker theorem. Selected topics from integer programming, network flows, transportation problems, inventory problems, and other applications. Three lectures, one recitation. *Prerequisites: Math. 20F and knowledge of programming.*

MATH 172 Numerical Partial Differential Equations (4)
Finite difference methods for the numerical solution of hyperbolic and parabolic partial differential equations; finite difference and finite element methods for elliptic partial differential equations. Three lectures. *Prerequisites: Math. 170A or Math. 110 and programming experience. (S)*

MATH 176. Advanced Data Structures (4)
Floating point arithmetic, linear equations, interpolation, integration, differential equations, nonlinear equations, optimization, least squares. *Prerequisites: Math 2-D (21D) and Math 20F*

MATH 173 Mathematical Software-Scientific Programming (4)
Development of high quality mathematical software for the computer solution of mathematical problems. Three lectures, one recitation. *Prerequisites: Math. 170A or Math. 174 and knowledge of FORTRAN. (W)*

MATH 210A Mathematical Methods in Physics and Engineering (4)

Complex variables with applications. Analytic functions, Cauchy's theorem, Taylor and Laurent series, residue theorem and contour integration techniques, analytic continuation, argument principle, conformal mapping, potential theory, asymptotic expansions, method of steepest descent. *Prerequisites: Math. 20DEF, 140A/142A or consent of instructor.*

MATH 210B Mathematical Methods in Physics and Engineering (4)
Linear algebra and functional analysis. Vector spaces, orthonormal bases, linear operators and matrices, eigenvalues and diagonalization, least squares approximation, infinite-dimensional spaces, completeness, integral equations, spectral theory, Green's functions, distributions, Fourier transform. Math. 210A or consent of instructor. (W) *Prerequisites: None*

MATH 210C Mathematical Methods in Physics and Engineering (4)
Calculus of variations: Euler-Lagrange equations, Noether's theorem. Fourier analysis of functions and distributions in several variables. Partial differential equations: Laplace, wave, and heat equations; fundamental solutions (Green's functions); well-posed problems. Math. 210B or consent of instructor. (S) *Prerequisites: None*

MATH 212A Introduction to the Mathematics of Systems and Control (4)
Linear and nonlinear systems, and their input-output behavior, linear continuous time and discrete-time systems, reachability and controllability for linear systems, feedback and stabilization, eigenvalue placement, nonlinear controllability, feedback linearization, disturbance rejection, nonlinear stabilization, Lyapunov and control-Lyapunov functions, linearization principle for stability. *Prerequisites: Math. 102 or equivalent, Math. 120A or equivalent, Math. 142A or equivalent*.

MATH 212B Introduction to the Mathematics of Systems and Control (4)
Observability notions, linearization principle for observability. Realization theory for linear systems, observers and dynamic feedback, detectability, external stability for linear systems, frequency-domain considerations, dynamic programming, quadratic cost, state estimation and Kalman filtering, nonlinear stabilizing optimal controls, calculus of variations, and the Maximum Principle. Math. 212A. *Prerequisites: None*

MATH 212C Introduction to the Mathematics of Systems and Control (4)
Topics of current interest on systems theory, control, and estimation to be chosen by instructor. Math. 212B. *Prerequisites: None*

MATH 270A-B-C Numerical Mathematics (4-4-4)
Error analysis of the numerical solution of linear equations and least squares problems for the full rank and rank deficient cases. Error analysis of numerical methods for eigenvalue problems and singular value problems. Error analysis of numerical quadrature and of the numerical solution of ordinary differential equations. *Prerequisites: Math. 20F and knowledge of programming.*

MATH 271A-B-C Numerical Optimization (4-4-4)
Formulation and analysis of algorithms for constrained optimization. Optimality conditions; linear and quadratic programming; interior methods; penalty and barrier function methods;

sequential quadratic programming methods. consent of instructor. (F,W,S) *Prerequisites: None*

MATH 272A-B-C Numerical Partial Differential Equations (4-4-4)
The numerical solution of elliptic, parabolic, and hyperbolic partial differential equations; discretization and solution techniques. consent of instructor. (F,W,S) *Prerequisites: None*

MATH 273A-B-C Scientific Computation (4-4-4)
Continuum mechanics models of physical and biological systems, finite element methods and approximation theory, complexity of iterative methods for linear and nonlinear equations, continuation methods, adaptive methods, parallel computing, and scientific visualization. Project-oriented; theoretical and software development projects designed around problems of current interest in science and engineering. experience with Matlab and C, some background in numerical analysis, or consent of instructor. (F,W,S) *Prerequisites: None*

MATH 277A Topics in Numerical Mathematics (4)
Topics vary from year to year. May be repeated for credit with consent of adviser. consent of instructor. *Prerequisites: None*

MATH 278 Seminar in Numerical Mathematics (1 to 4)
Consent of instructor. (S/U grades permitted.) *Prerequisites: None*

MATH 294 The Mathematics of Finance (4)
Introduction to the mathematics of financial models. Hedging, pricing by arbitrage. Discrete and continuous stochastic models. Martingales. Brownian motion, stochastic calculus. Black-Scholes model, adaptations to dividend paying equities, currencies and coupon-paying bonds, interest rate market, foreign exchange models. *Prerequisites: Math. 180A (or equivalent probability course) or consent of instructor.*

Mechanical and Aerospace Engineering:
MAE 107. Computational Methods in Engineering (4) Introduction to scientific computing and algorithms; iterative methods, systems of linear equations with applications; nonlinear algebraic equations; function interpolation and differentiation and optimal procedures; data fitting and least-squares; numerical solution of ordinary differential equations. *Prerequisites: engineering majors only and grades of C\u2013 or better in MAE 9 or MAE 10 and Math. 20F.*

MAE 223. Computational Fluid Dynamics (4) Numerical methods in fluid dynamics and convective transport processes. Numerical solution of the Euler and Navier-Stokes equation. Additional topics will vary according to instructor. Examples include eigenvalue problems in hydrodynamic stability, vortex methods, spectral and panel methods. *Prerequisite: MAE 210A, 210B, 290A-B or equivalent.*

MAE 232A. Finite Element Methods in Solid Mechanics I (4) Finite element methods for linear problems in solid mechanics. Emphasis on the principle of virtual work, finite element stiffness matrices, various finite element formulations and their accuracy and the numerical implementation required to solve problems in small strain, isotropic elasticity in solid mechanics. *Prerequisite: graduate standing.*

MAE 232B. Finite Element Methods in Solid Mechanics II (4) Finite element methods for linear problems in structural dynamics. Beam, plate, and doubly curved shell elements are derived. Strategies for eliminating shear locking problems are introducted. Formulation and numerical solution of the equations of motion for structural dynamics are introduced and the effect of different mass matrix formulations on the solution accuracy is explored. *Prerequisites: graduate standing and MAE 230 or MAE 232A.*

MAE 249. Advances in Materials Computations (4) This course will cover nonlinear finite element methods in large deformations and nonlinear materials. Particular emphasis will be placed on material models that are appropriate for high strain rates, high pressures, and phase transformations. *Prerequisites: MAE 231A, 232A.*

MAE 280A. Linear Systems Theory (4) Linear algebra: inner products, outer products, vector norms, matrix norms, least squares problems, Jordan forms, coordinate transformations, positive definite matrices, etc. Properties of linear dynamic systems described by ODEs: observability, controllability, detectability, stabilizability, trackability, optimality. Control systems design: state estimation, pole assignment, linear quadratic control. *Prerequisite: MAE 141A or 143B, or consent of instructor.*

MAE 280B. Linear Control Design (4) Parametrization of all stabilizing output feedback controllers, covariance controllers, H-infinity controllers, and L-2 to L-infinity controllers. Continuous and discrete-time treatment. Alternating projection algorithms for solving output feedback problems. Model reduction. All control design problems reduced to one critical theorem in linear algebra. *Prerequisite: MAE 280A.*

MAE 290A. Numerical Methods in Science and Engineering (4) A general introductory course to numerical methods. Introduction to linear calculus, solution of systems of linear and nonlinear algebraic equations, the algebraic eigenvalue problem, polynomial and trigonometric function interpolation, function differentiation and integration, function approximation. *Prerequisite: MAE 107 or consent of instructor.*

MAE 290B. Numerical Methods for Differential Equations (4) Numerical solution of differential equations in mathematical physics and engineering, ordinary and partial differential equations. Linear and nonlinear hyperbolic parabolic, and elliptic equations, with emphasis on prototypical cases, the convection-diffusion equation, Laplace\u2019s and Poisson equation. Finite difference methods will be considered in depth, and additional topics. *Prerequisite: MAE 290A or consent of instructor.*

MAE 293. Advanced Computer Graphics for Engineers and Scientists (4) Advanced topics used to enhance scientific and engineering visualization. C programming assignments and the use of advanced graphics software. Continuation of topics from MAE 152, including color, computational geometry, 3-D contouring, volume visualization, and hardware architectures. *Prerequisite: MAE 152 or consent of instructor.*

MAE 294A. Methods in Applied Mechanics I (4) Solution of linear and nonlinear ordinary differential equations: initial-valve and boundary-valve problems, classifications of ordinary and singular points, regular and asymptotic series solutions, phase-plane analysis, regular and singular perturbation theory, asymptotic expansions and multiscale analyses. Applications to the dynamics of mechanical, chemical, and biological systems. *Prerequisite: Math. 110, Math.120A, or consent of instructor.*

MAE 294B. Methods in Applied Mechanics II (4) Complex variables, asymptotic expansions of integrals, steepest descents and stationary phase, Fourier series and Fourier transforms, boundary-layer theory, the WKBJ method, matched asymptotic expansions. Applications to fluid mechanics, hydrodynamics, and gas dynamics. *Prerequisite: MAE 294A or consent of instructor.*

MAE 294C. Methods in Applied Mechanics III (4) Partial differential equations and boundary-value problems, classification of PDE's and transform methods. Green's functions and spectral theory. Nonlinear PDE's, variational methods and the methods of characteristics. Nonlinear waves and shocks. Asymptotic methods for PDE's. Galerkin methods and numerical analysis of PDE's. Applications to continuum mechanics and transport phenomena. *Prerequisite: MAE 294B or consent of instructor.*

Physics:

PHYS 105A. Mathematical and Computational Physics (4)
A combined analytic and mathematica-based numerical approach to the solution of common applied mathematics problems in physics and engineering. Topics: Fourier series and integrals, special functions, initial and boundary value problems, Green’s functions; heat, Laplace and wave equations. *Prerequisites: Mathematics 20E and 20F and Physics 4E or 2D.* (F)

PHYS 105B. Mathematical and Computational Physics (4)
A continuation of Physics 105A covering selected advanced topics in applied mathematical and numerical methods. Topics include statistics, diffusion and Monte-Carlo simulations; Laplace equation and numerical methods for nonseparable geometries; waves in inhomogeneous media, WKB analysis; nonlinear systems and chaos. *Prerequisite: Physics 105A.* (W)

PHYS 141/241.Computational Physics I: Probabilistic Models and Simulations (4)
Project-based computational physics laboratory course with student’s choice of Fortran90/95, or C/C++. Applications from materials science to the structure of the early universe are chosen from molecular dynamics, classical and quantum Monte Carlo methods, physical Langevin/Fokker-Planck processes, and other modern topics. *Prerequisite: upper-division standing or consent of instructor.* (W)

PHYS 142/242. Computational Physics II: PDE and Matrix Models (4)
Project-based computational physics laboratory course for modern physics and engineering problems with student’s choice of Fortran90/95, or C/C++. Applications of finite element PDE models are chosen from quantum mechanics and nanodevices, fluid dynamics, electromagnetism, materials physics, and other modern topics. *Prerequisite: upper-division standing or consent of instructor.* (S)

PHYS 221A. Nonlinear and Nonequilibrium Dynamics of Physical Systems (4)
An introduction to the modern theory of dynamical systems and applications thereof. Topics include maps and flows, bifurcation theory and normal form analysis, chaotic attractors in dissipative systems, Hamiltonian dynamics and the KAM theorem and time series analysis. *Prerequisites: Physics 200B (W)*

PHYS 221B. Nonlinear and Nonequilibrium Dynamics of Physical Systems (4)
Nonlinear dynamics in spatially extended systems. Material to be covered includes fluid mechanical instabilities, the amplititude equation approach to pattern formation, reaction-diffusion dynamics, integrable systems and solitons and an introduction to coherent structures and spatio-temporal chaos. *Prerequisites: Physics 210B and 221A (S)*

PHYS 225A-B. General Relativity (4-4) This is a two-quarter course on gravitation and the general theory of relativity. The first quarter is intended to be offered every year and may be taken independently of the second quarter. The second quarter will be offered in alternate years. Topics covered in the first quarter include special relativity, differential geometry, the equivalence principle, the Einstein field equations, and experimental and observational tests of gravitation theories. The second quarter will focus on more advanced topics, including gravitational collapse, Schwarzschild and Kerr geometries, black holes, gravitational radiation, cosmology, and quantum gravitation. (225B offered in alternate years) (F,W)

Structural Engineering:
SE 201. Advanced Structural Analysis (4) Applications of advanced analytical concepts to structural engineering problems. Effects of approximations in the descretization and the type of finite elements under consideration. An introduction is given to the nonlinear behavior of structural systems focusing on basic concepts and computational techniques. *Prerequisites: SE 130A-B or equivalent, or consent of instructor.*

SE 222. Geotechnical Earthquake Engineering (4) Influence of soil conditions on ground motion characteristics; dynamic behavior of soils, computation of ground response using wave propagation analysis and finite element analysis; evaluation and mitigation of soil liquefaction; soil-structure interaction; lateral pressures on earth retaining structures; analysis of slope stability

SE 223. Advanced Seismic Design of Structures (4) Introduction to fundamental concepts in seismic design of structures. Ductility. Elastic and inelastic response. Time-history analysis. Response spectral analysis. Force- and displacement-based design. Capacity design principles. Learning from earthquake damage. Performance-based design concepts.

SE 234. Plates and Shells (4) General mathematical formulation of the theory of thin elastic shells; linear membrane and bending theories; finite strain and rotation theories; shells of revolution; shallow shells; selected static and dynamic problems; survey of recent advances.

SE 244. Numerical Methods in Geomechanics (4) Application of the finite element method to static and dynamic analysis of geotechnical structures. One-, 2-, and 3-D seismic site response of earth structures and slopes. Pore-pressure generation and effects during cyclic loading. System identification using strong motion array data.

SE 245. Constitutive Modeling and Numerical Implementation (4) Development and numerical implementation of procedures to model the nonlinear behavior of engineering materials, including soil and concrete. Inelastic hyperbolic and elasto-plastic modeling of hysteretic response to cyclic loading. Behavior of soil-structure systems under transient loading, such as seismic earthquake excitation, will be discussed.

5.2 Proposed New Courses

Chemistry:

CHEM 288 Topics in Contemporary Computational Biology (4)
This course will focus on discussing several important topics in the contemporary computational biology and bioinformatics. Topics will include inference of gene modules, reconstructing gene regulatory networks and prediction of signal transduction network. The algorithms that will be discussed in the course include Bayesian network, hidden Markov model (HMM), Markov chain Monte Carlo, Gibbs sampling and expectation maximization (EM).

CHEM 184 Computational Biology (4)
This course will introduce the computational issues and methods used in molecular and systems biology, combining core lectures, homework assignments, programming projects with midterm and final exams. The course will introduce and use biological data sources available on the World Wide Web media. Topics will include detection of DNA and protein sequence patterns, analysis of DNA microarray data, inference of gene regulatory networks, prediction of protein structure and protein interaction partners, identification of network motifs. The algorithms that will be introduced in the course include, for example, hierarchical clustering, k-mean clustering, structural superposition algorithms, protein motif definition and identifiction.

Mathematics:

MATH 174/274 Numerical Methods in Science and Engineering (4)
Floating point arithmetic, direct and iterative solution of linear systems of equations, iterative solution of nonlinear equations, optimization, approximation theory, interpolation, quadrature, numerical integration of initial value and boundary value problems in ordinary differential equations. *Prerequisites: None*

MATH 275 Numerical Methods for Partial Differential Equations (4)
Basic mathematical background in partial differential equations (PDE) of elliptic, parabolic, and hyperbolic type. Survey of finite different, finite volume, finite element, and spectral methods for the discretization of PDE. Basic techniques in error estimation and adaptivity. *Prerequisites: None*

Physics:

PHYS 243 Stochastic Methods (4)

Introduction to methods of stochastic modeling and simulation. Topics include: random variables; stochastic processes; Markov processes; one-step processes; the Fokker-Planck equation and Brownian motion; the Langevin approach; Monte-Carlo methods; fluctuations and the Boltzmann equation; and stochastic differential equations. *Prerequisites: calculus and elementary probability*

PHYS 244 Parallel Computing in Science and Engineering (4)
Introduction to the basic techniques of parallel computing, the choice and design of parallel algorithms and their scientific and engineering applications. Topics include: parallel computing platforms; MPI: the paradigm of parallel software; design and application of parallel software packages; parallel visualization; parallel scientific applications; and parallel engineering applications. *Prerequisites: Calculus and basic programming proficiency. Knowledge of numerical analysis and numerics of PDEs. Basic knowledge in physics and chemistry*.

6.0 RESOURCES

The necessary resources to launch this program have been identified and are described below. Commitments to provide the funding are documented in Appendices C.1 and C.2.

6.1 Faculty FTE

We currently have the critical mass of faculty necessary to serve this program. This was facilitated by the recent appointments of Drs. Li-Tien Chen, Bo Li and Glenn Tesler in the Department of Mathematics; Dr. Wei Wang in the Department of Chemistry and Biochemistry and Drs. Massimilliano DiVentra and Paolo Padoan in the Department of Physics.

Designated committee faculty members will commit time and effort to this program. A course reduction for the Director(s) is in order given the significant responsibility and administrative effort required.

6.2 Library Acquisition – None

6.3 Computing

Our plan calls for two computing labs. “Lab A” is an existing computing lab in the Department of Physics which will be made available to this program. Through an investment by the Division of Physical Sciences, some computing upgrades have recently taken place. However, Lab A will require the replacement of the 22 workstations in the second year of the new program at an estimated cost of $60K. In order to meet the needs of the new graduate program, we would also install a small low cost blade system of four, or eight nodes ($10K) where the students can practice parallel computing in the lab projects. In addition, $30K will be spent on the substantial improvement of the communication infrastructure in the lab. The proposed structural change would include a dedicated server located in Academic Computing and a mirror server in the lab with nightly mirroring of the ACS server. This will both improve performance of Lab A, as well as cut down on bandwidth load on the campus backbone between Urey Hall and the ACS servers in AP&M.

New ASF for “Lab B” has been requested. Our plan is to build a computational science laboratory consisting of 32 graphics workstations supported by 2 fileservers, a separate 32-node blade-type Beowulf cluster and a dedicated 9-node visualization cluster. The graphics workstations will run a version of Linux and will contain NVIDIA graphics hardware for use with OpenGL-based visualization tools. The 32-node Beowulf cluster will run SDSC’s locally developed NPACI/ROCKS clustering software. The 9-node dedicated visualization cluster will also run the NPACI/ROCKS software, but will also be configured with high-end NVIDIA graphics hardware and the ROCKS Visualization Roll. This 9-node cluster will drive a 9-panel visualization wall. The workstations, Beowulf cluster, and visualization cluster will provide a state-of-the-art training platform for the parallel computing, visualization, and application-specific computational science courses that support the graduate program. This computational laboratory is critical to the success of the graduate program. The estimated cost of the entire laboratory, including supporting networking, power, and related infrastructure, is $400,000. We should anticipate upgrades and/or replacements on a 4-5 year cycle. The most costly component of the laboratory will be the acquisition of the Beowulf cluster; we have included a representative quote from a well-regarded blade vendor as an estimate of these costs. The Dean of Physical Sciences will provide funding for the labs as indicated in Appendix C.1.

6.4 Equipment

See 6.3 above.

6.5 Space and Capital Facilities

Space to accommodate the CSME Program has been made available in the Applied Mathematics and Physics Building. The commitment of space is documented in Appendix C.2.

6.6 Other Operating Costs

Additional new costs are minimal given the effort to leverage existing resources in the Division of Physical Sciences – particularly those that exist in the Department of Mathematics. We anticipate a small one-time start-up cost for furnishings and staff computing. Recurring, permanent costs include the provision of 1.00 staff FTE of which 0.50 FTE will focus on administrative support and 0.50 FTE to serve as a programmer/analyst. The necessary funding will be provided by the Dean of Physical Sciences and the Sr. Vice Chancellor, Academic Affairs as documented in Appendices C.1 and C.2.

7.0 GRADUATE STUDENT SUPPORT

All Ph.D. students will be admitted through a home department that will be responsible for providing funding according to procedures in place in respective departments. Our resource plan includes an extensive effort to identify external resources in support of graduate students.

8.0 CHANGES IN SENATE REGULATIONS

None required

APPENDICES

A. Departmental Participation Agreements
B. Faculty CVs
C. Letters of Commitment
    1. Dean of Physical Sciences
    2. Sr. Vice Chancellor, Academic Affairs