

PROPOSAL FOR AN INTERDISCIPLINARY CENTER FOR SCIENTIFIC COMPUTING

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Scientific computing enhances our understanding of such diverse topics as the cosmos, genomics, the atmosphere and oceans, biodiversity, aerodynamics, forest fires, and the weather. The increased use of computational methods in the sciences presents us with three challenges: the need for powerful hardware, efficient software, and the expertise in numerical methods. The Interdisciplinary Center for Scientific Computing will meet these challenges by creating an interdisciplinary environment for scientists and computational mathematicians to collaborate on scientific problems requiring computational tools, and providing high quality computational resources and software.

1 Scientific Computing

The last few decades have seen a dramatic increase in the speed and data handling capability of high performance computers, and the development of novel algorithms, which together have transformed scientific investigation. Scientific computation has joined experiment and theory, and has become central to scientific development and discovery. Large scale computational algorithms are utilized in virtually every scientific field. In biology, examples include the determination of protein structures from data given by nuclear magnetic resonance, x-ray crystallography, or electron microscopy, parallel computation of protein folding models and biomolecular dynamics simulations, and simulation of biological processes. Chemists use computing techniques extensively in spectroscopy, molecular modeling of organic and inorganic molecules, quantum chemical calculations, molecular dynamics and mechanics, and drug discovery. In physics, astrophysical and oceanographic models are simulated using some of the most advanced and complex numerical algorithms. Weather prediction is based on the numerical simulation of weather models. Engineers are by far the most sophisticated users of scientific computing, and applications such as computational fluid dynamics and image processing require extensive computational time and memory, and yield high level information for a wide variety of applications.

The increased importance of computing in the sciences poses new challenges, as well. The first challenge is the availability and efficient use of computational facilities. Scientists need a parallel cluster of workstations to perform numerical simulations, and these computers need to be efficiently configured and connected. The computational resources must also be used efficiently; this is not possible when the same machine must serve as a personal computer and workstation. The second challenge is in providing the appropriate software for the problem. There are many commercial as well as free software packages available for a large variety of problems. It is necessary to identify the appropriate software packages and make them available for use by science and engineering faculty and their graduate students. The third challenge is in providing the numerical analysts, experts in numerical methods who can direct and advise scientists on the use and limitations of numerical methods and innovate and develop new numerical methods tailored to a given scientific problem.

2 Goals and Vision

The UMass Interdisciplinary Center for Scientific Computing (ICSC) will meet the challenges of the era of scientific computing by providing scientists with the hardware and software needed for numerical simulations, as well as enabling collaborations between the scientists and the numerical analysts. These collaborations will foster research activities that develop and utilize novel computational algorithms to aid scientific discovery.

1. **Hardware:** The ICSC will house a cluster of parallel workstations, which will be available for numerical simulations.

Powerful workstations have become affordable in recent years, but are significantly more expensive than a desktop personal computer. These machines cannot be used efficiently if they are concurrently used for email, and internet and word-processing applications. It is essential that the machines be solely dedicated to running numerical simulations. Furthermore, parallel computing is needed for simulations which have large scale computation, data, and storage needs. For this, we require a parallel computer, or we can combine several workstations into a parallel cluster of computers. The ICSC will begin with a cluster of eight workstations, which can be used separately, or combined as a parallel cluster, depending on the simulation.

2. **Software** The ICSC will provide reliable software for scientific computing.

The affiliates of the center will identify efficient software, which will be installed and tested on the workstations in the center. The ICSC has affiliates who have the expertise to advise users on each package's use and its limitations. This will prevent the computer and human time loss which results from using an application that is ill-suited to a problem. There are many software packages available for scientific computing, a few examples include:

HPF: The High Performance Fortran Forum (HPFF), a coalition of industry, academic and laboratory representatives, works to define a set of extensions to Fortran 90 known collectively as High Performance Fortran (HPF). HPF extensions provide access to high-performance architecture features while maintaining portability across platforms.

PETSc is a suite of data structures and routines for the scalable (parallel) solution of scientific applications modeled by partial differential equations. This software is freely available.

FLUENT is a finite volume based, commercially available computational fluid dynamics software.

PseudoPack (2000) is a freely available support package for spectral methods codes for solution of partial differential equations, and provides subroutines for performing basic operations such as generation of proper collocation points, differentiation and filtering matrices.

USEMe is an unstructured spectral element method code, which can be obtained from the author at no cost. It is designed for simulations of electromagnetics, fluid dynamics, and plasma dynamics. It can be implemented in parallel or serial.

GAUSSIAN is software for molecular modeling and chemical reaction dynamics, developed by Gaussian Inc.

MOLGEN is an efficient and portable tool for molecular structure elucidation for chemical research.

Molpro is a complete system of ab initio programs for molecular electronic structure calculations.

MSI software by Molecular Simulations Inc. for homology modeling and dynamics software (this software is extremely expensive and would not be purchased until the need and funding arises).

PredictProtein is a free service for sequence analysis, and structure prediction.

PSI is a free package of ab initio quantum chemistry software developed at the center for computational chemistry at the University of Georgia.

X-PLOR and **CNSsolve** are programs for structure determination from data obtained by x-ray crystallography and nuclear magnetic resonance. They are free to academic institutions.

Additionally, there is software necessary for visualization, and there are problems for which there is no available software and the codes must be written by numerical analysts.

Although some of the software must be purchased, a lot of it is freely available. However, unlike the software we use for everyday applications on a personal computer, this software is not self extracting and installing! Software must be downloaded and installed. Proper installation and maintenance is

essential to assure that programs run properly in parallel. The technician will be able to support linux based computers outside of the center, which are being used for research by our affiliates. Currently there is little or no support on campus for linux based research computers on our campus.

3. **Human Expertise: Collaboration and Innovation:** The ICSC hardware and software resources will be significant, but the most valuable aspect of the center is the human capital, the ICSC affiliates.

The ICSC's affiliates are scientists and applied mathematicians. We typically classify the scientists as experts in the physical problem, and the applied mathematicians as experts in the numerical methods. However, the ICSC affiliates have significant experience in both aspects of numerical simulation. The ICSC will bring together scientists in many fields as well as mathematicians, and the impact on each field will be greater than the sum of its parts.

On its most basic level, the center will bring together the scientist and computational mathematician to identify numerical methodologies for the simulation of a given model. They will determine whether there are software packages which can be used for a given simulation, whether additional software is available for parts of the code which need to be written, or whether they must develop new code. This type of collaborative environment has not previously been available at UMass Dartmouth, and scientists interested in numerical methods typically have not sought or received support from an experts in numerical methods. In some cases this may have led to inappropriate choices of software for a given problem or choices of parameters or options that were far from optimal. High performance computing requires an understanding of the underlying numerical methods as well as the parallel structure of the method. These are topics in which numerical analysts are experts, and the ICSC will make this expertise available to a wide variety of scientists. There are many scientists who have, through training as well as years of experience and numerical experimentation, developed significant expertise in the use and function of numerical methods, and these scientists will share their expertise with other scientists as ICSC affiliates.

These technical collaborations will provide a springboard for more innovative collaborations. Once a physical problem is identified, the scientist and numerical analyst may realize that it is necessary to tailor a numerical method for simulation of the problem, or perhaps create a new numerical method for the problem. This will lead to a collaboration which is innovative in both the physical and mathematical aspects. The opportunity for such collaborations is important to both scientists and applied mathematicians, and the ICSC will provide the setting for truly innovative collaborative research.

The center will be headed by two directors: Sigal Gottlieb and Steven J. Leon. The affiliates of the ICSC will be numerical analysts, engineers, physical scientists, computer scientists, and biological scientists. The affiliates will serve on a board of directors, which will guide the center's development and direction. A graduate student will be funded as a technician and coordinator of the center. Her/his responsibilities will include management of the workstations, downloading and testing of software, and setting up a website for the center.

3 Affiliates of the Center

Although the need for computational resources is critical for the existence of the center, its excellence will depend on its affiliates.

Ramprasad Balasubramanian (*Computer and Information Sciences*): Computer Vision, Image Processing, Artificial Intelligence and HCI

James Bisagni (*Marine Sciences*): Global Ecosystems Dynamics.

Changsheng Chen (*Marine Sciences*): Ecosystems Dynamics Modeling.

Chi Hau Chen (*Electrical and Computer Engineering*): Image Processing, Machine Vision.

Alex Fowler (*Mechanical Engineering*): Fluid Flow in Porous Media, Heat Transfer, Thermodynamics, Bioengineering.

David Goodson (*Chemistry*): Quantum Chemistry Methods Development, Quantum Molecular Dynamics.

Sigal Gottlieb (*Mathematics*): Numerical Analysis, Shock Wave Calculation, WENO methods, Gibbs phenomenon removal.

Jong-Ping Hsu (*Physics*): Theoretical Physics: symmetry principles and gauge field theories.

Jae-Hun Jung (*Mathematics*): Numerical Analysis, Spectral Methods, Gibbs phenomenon removal. (New faculty)

Dayalan Kasilingam (*Electrical and Computer Engineering*): Remote Sensing, Applied Electromagnetics, Wireless Communications, Adaptive Signal Processing.

Gaurav Khanna (*Physics*): Theoretical and Computational Astrophysics, Black Hole Astrophysics, Gravitational Waves, Quantum Gravity, High-Performance Computing, Control and Dynamical System Theory.

Raymond Laoulache (*Mechanical Engineering*): Thermodynamics, Multiphase Flow, Control Systems, Fluid Mechanics, Laser Doppler Anemometry, Parallel Computing.

Steven J. Leon (*Mathematics*): Numerical Analysis, Matrix Computations.

Steven C. Nardone (*Electrical and Computer Engineering*): Systems Theory, Control and Estimation Theory, Fuzzy Systems, Applications to Target Tracking.

Eli Stahl (*Biology*): Molecular Population Genetics, Population Structure, Conservation Genetics, Molecular Evolution, Disease Resistance.

Timothy C. Su (*Chemistry and Biochemistry*): Ion Chemistry, Mass Spectrometry, Computational Chemistry, Drug Discovery.

Amit Tandon (*Physics*): Physical Oceanography, Fluid Dynamics, Computational Physics, Motion Analysis and Visualization.

Marguerite Zarillo (*Physics*): Transportation Engineering, traffic simulation, modeling and computing.

4 Budget

The amounts budgeted will enable the ICSC to run for three years, which will be enough time to allow it to become self-supporting through grants. The expenses for the first year include hardware and software costs. Faculty release time and sabbatical leave funds will allow the directors of the center to devote their time to the establishment and development of the center, especially the task of getting grants which will support the center.

Year 1	Hardware	8 linux workstations	\$45,000
	Software		\$12,000
Year 2	1 Faculty	Course release	\$10,000
	1 Faculty	Sabbatical leave	\$33,000
	Coordinator/Technician	part-time	\$25,000
Year 3	3 Faculty	Course releases	\$27,000
	Coordinator/Technician	part-time	\$25,000
Year 3	3 Faculty	Course releases	\$27,000
	Coordinator/Technician	part-time	\$25,000
Total			\$ 229,000

5 Plan for Future Funding

The ICSC will become self-sufficient within three years. Its growth will depend on federal grants made for the center itself, as well as research grants made to affiliates of the center, to support research at the center. These grants will pay for additional computational resources, for the funding of a technician, and for new and upgraded software.

6 Benefits of a Scientific Computing Center

A scientific computing center will have significant benefits to UMass Dartmouth and to the entire UMass system. There will also be significant benefits to the Southcoast region and to the Commonwealth, as well as national benefits.

1. **UMass Dartmouth and the UMass System.** The interdisciplinary collaborations fostered through the ICSC will lead to more sophisticated computational models which will in turn lead to improved research results. Since interdisciplinary projects tend to be broader in scope, they are generally funded at a higher level. The increased funding the ICSC brings in can be used to further support research at the university. Graduate students will also benefit from the improved facilities for doing modeling and simulations and from the opportunities to work on interdisciplinary projects and to consult with experts on numerical computations.

Once the center is up and running we plan to make it accessible to faculty at our sister UMass campuses. Thus the center will not only facilitate interdisciplinary research, but also intercampus collaborations. The whole system will benefit.

2. **The Southcoast region and the Commonwealth of Massachusetts.** Currently UMass Dartmouth faculty are actively involved in research that impacts local industries such as the fishing industry and the cranberry industry. Improved mathematical models and simulations in these fields will lead to improvements in harvesting and conservation that will have positive impact on the economy of the region. Through the ICSC our graduate students will be better trained for high tech jobs in the region and for government jobs at facilities such as the Naval Underwater Warfare Center in Newport.

Modern biological models are extremely complex and involve massive amounts of computation. The ICSC will provide the facilities for these computations and will help train students in biological modeling. Through both research and the training of researchers the center will contribute significantly to the build up of the biotech industry in Massachusetts. We will also train graduate students to help meet the staffing needs of the many high tech software companies in Massachusetts.

3. **The nation as a whole.** The ICSC will foster interdisciplinary research that will have a national impact. Working through the center, faculty will be able to form federal partnerships to help meet national goals. Improved mathematical models and simulations can lead to advances in health care, improvements in homeland security, better environmental models, improved structures and construction, etc. These partnerships are offered through programs in the departments of agriculture, defense, energy, transportation and through agencies such as the National Institute of Health, the National Science Foundation, the Environmental Protection Agency, and the National Oceanic and Atmospheric Administration.