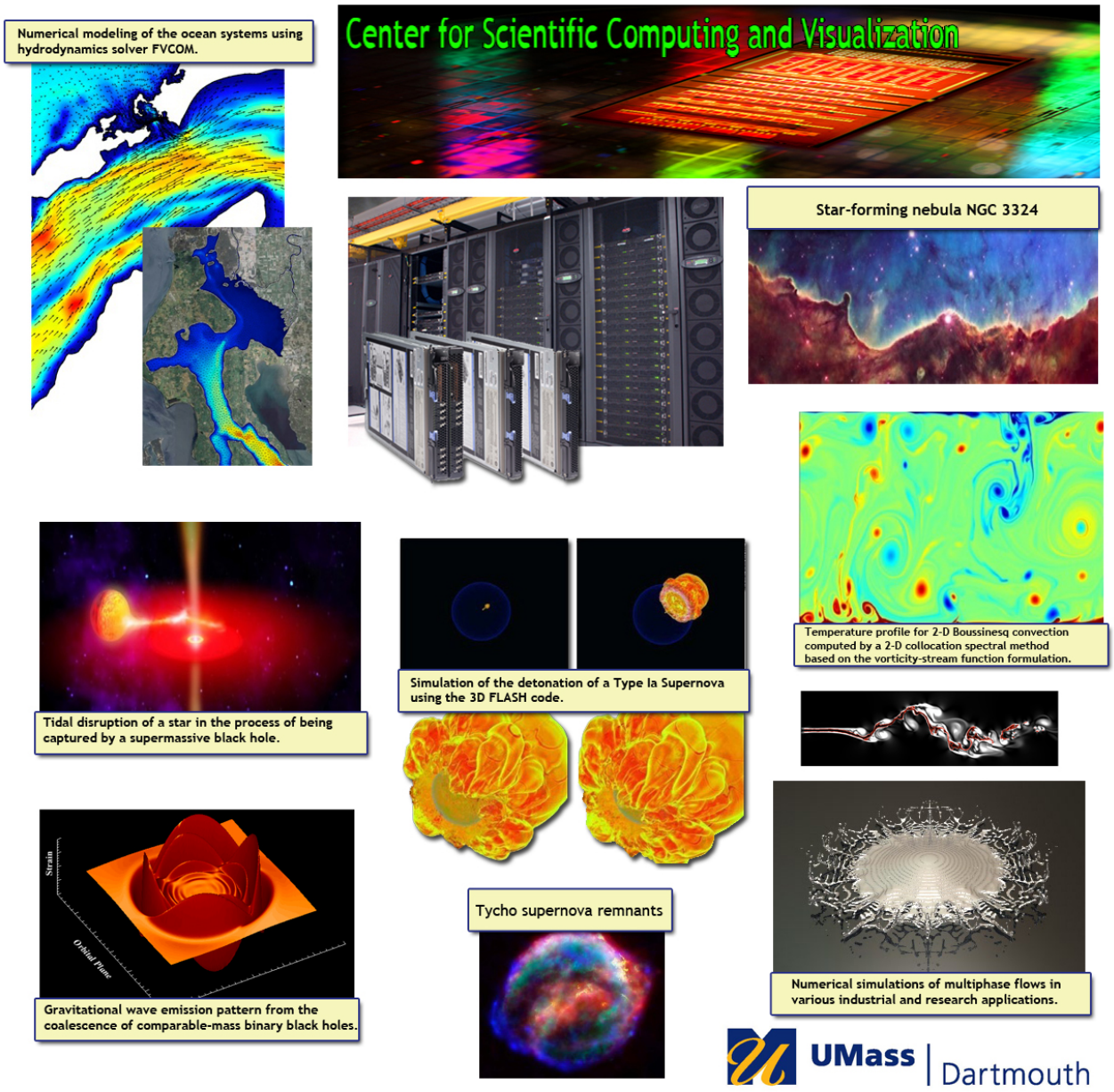

Proposal for a Center for Scientific Computing and Visualization at UMass Dartmouth

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By the Scientific Computing Group

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1 Description of the proposed Center

The UMass Dartmouth Center for Scientific Computing and Visualization will unite faculty members from across campus whose research and expertise is in scientific computing, and leverage the existing multidisciplinary and interdisciplinary strengths in scientific computing to build an internationally recognized center of excellence at UMass Dartmouth.

2 Purpose and activities of the Center

2.1 Mission

The mission of the proposed Center is to promote and conduct high-level interdisciplinary and multidisciplinary research in scientific computing, and to mentor students of scientific computing - school students, undergraduates, and graduate students - in a supportive, broad, and deep interdisciplinary research environment. The Center for Scientific Computing and Visualization will support, facilitate, and advertise the activities of the scientific computing group, which is comprised of over a dozen researchers from Mechanical and Civil Engineering, Mathematics, Physics and SMAST who develop and use computational algorithms to simulate complex physical problems, and visualize these solutions using pictures and movies. The Center will support faculty research and work closely with IT to keep UMass Dartmouth at the forefront of high performance computing and visualization. Through seminars and workshops, the Center will foster collaborative research within the group and between the members of the scientific computing group and researchers at other Universities, National Labs, and Industry, and enhance the reputation of the University of Massachusetts Dartmouth.

2.2 Rationale

The dramatic increase in the speed and data-handling capability of high performance computers (HPCs), and a complementary development of novel algorithms, have over the past few decades transformed the nature of scientific investigation. Computation is now used regularly and intensively for the simulation of complex physical problems such as climate modeling, weather prediction, design of airplanes and engines, and the study of star formation and supernova, among many others. The results of these computations are visualized in movies and pictures, which is central to the process of obtaining insights about the physical phenomena studied. *Scientific computation has joined experiment and theory to become a central pillar of modern science.*

Across campus, faculty members from a variety of Departments and Colleges have formed an active scientific computing group. This is a multidisciplinary and interdisciplinary group, made up of highly-qualified and well-trained scientists with complementary backgrounds and interests who develop and use computational algorithms to simulate and visualize complex physical problems. This expertise in scientific computing transcends the traditional boundaries of academic field or department, and has led to joint seminars, research collaborations, submitted and funded proposals to Federal agencies, co-advising of students, and the development of a multidisciplinary doctoral program.

The creation of a Center for Scientific Computing and Visualization will provide multiple benefits to the faculty of the scientific computing group and to the University. The Center

will focus on developing and applying unique and powerful computation tools to address pressing scientific and societal challenges currently being studied by the members of the scientific computing group. By providing a unified focal point for scientific computing, the Center will highlight the accomplishments of many scientists across campus, provide support and collaboration opportunities within and out of campus, and establish UMass Dartmouth as an active center of excellence in the computational sciences. This will, in turn, make UMass Dartmouth scientists more competitive in obtaining external funding, will enhance the retention of faculty in scientific computing and make the University more attractive to future hires. In this way, the Center will further Research Strategic Plan of the University.

Through its educational efforts, the Center will provide a focal point for inter and multi-disciplinary research projects for undergraduate and graduate students. Our students will be offered a unique and transformative experience by being part of a strong and diverse scientific computing group which spans several academic disciplines.

Through the activities of the Center the University will advance its mission – by raising its research profile on the national and international level, by increasing external research revenues, and by providing high-quality discovery-based educational experiences for undergraduate as well as M.S. and Ph.D. graduate students.

2.3 Goals and Objectives

The major goals of the proposed Center are

1. To provide focus and support for scientific computing at UMass Dartmouth.
2. To establish the reputation of UMass Dartmouth as a world-class Center of excellence in scientific computing.
3. To seek collaborative external funding and research opportunities.
4. To educate and mentor the next generation of researchers in the computational sciences.

The activities of the Center will focus on building strong internal collaborative contacts within the scientific computing group, and bringing in scientists from other Universities, National Labs, and Companies with the aim of establishing external collaborations and broadcasting the accomplishments of the group.

2.4 Activities of the Center

The activities of the Center in support of research and education in scientific computing will include:

- Frequent seminars by external researchers in the computational sciences.
- Inviting and hosting visiting researchers for week-long visits for the purpose of establishing and maintaining external collaborations.
- Develop intensive international collaborations, utilizing such resources as videoconferencing and the proposed Digital Visualization Studio.

- Establishing and maintaining connections with other similar Centers around the country, and in particular with the NSF funded Institute for Computational and Experimental Research in Mathematics (ICERM) at Brown University, Center for Computation and Technology (CCT) at Louisiana State University (LSU) and the Information Directorate of the Air Force Research Lab (AFRL, Rome, NY).

- Engaging in emerging opportunities in the computational sciences which are in harmony with the research interests of Center affiliates, such as uncertainty quantification, data analysis, and computational biology and biomedical computing.

- Identifying mechanisms for seeking external funding.

- Assisting and supporting Center affiliates with proposal writing.

- Outreach to the wider scientific computing community through annual workshops.

- Developing existing and establishing new relations with computer industry R&D, such as IBM TJ Watson Research Center, Nvidia Research, Apple Inc.'s Advanced Computation Group (ACG) and others.

- Maintaining and managing available scientific computational infrastructure on campus, to keep Umass Dartmouth at the forefront of high performance computing and visualization.

- Mentoring students through an active, discovery-based approach to develop expertise in methods of scientific computing.

- Providing a focal point for scientific computing research in undergraduate education through the NSF funded CSUMS program

- Supporting and facilitating the new doctoral program track in the computational sciences.

- Establishing a consulting service, where industrial partners can be linked with Center affiliates and their students.

2.5 Future funding and growth potential

The strategy for future funding for the Center for Scientific Computing and Visualization relies on three approaches.

First, the affiliates of the Center will identify and collaborate on research grant opportunities, develop industry partnerships, and establish consulting services. Through these mechanisms the Center affiliates will bring in funding to the Center. The faculty members of the scientific computing group who will become affiliates of the Center have had significant success in obtaining grant funding, currently holding a total of $3M in external funds (see Section 3.4.1). The number of faculty members on campus with expertise in scientific computing has doubled in the last three years, and the group's success in obtaining external research funding is expected to rapidly increase in the next few years due to the recent hires of seven promising researchers in scientific computing. The Center affiliates are committed

to helping and mentoring new faculty in the process of writing grant proposals, which will increase the number and quality of proposals coming from the scientific computing group. The creation of a Center for Scientific Computing and Visualization will greatly enhance the competitiveness of the Center affiliates, and bring with it increased success in obtaining grant funding.

Second, the Center leadership will apply for bigger external grants appropriate for large-scale initiatives. In this way, the Center will bring in its own funding. The Center leadership will identify and apply for appropriate funding mechanisms for the Center itself, including such initiatives as

1. The Department of Energy's (Office of Advanced Scientific Computing Research) SciDAC program, which aims to fund scientific discovery through advanced computing institutes, at the level of $2M per annum.

2. The National Science Foundation's EMSW21 program, which works to enhance the mathematical sciences workforce, through grants of up to $3M.

3. The National Science Foundation's *Expeditions in Computing* program, which aims to provide up to $2M over 5 years to centers in Computer and Information Science and Engineering research and education, with the opportunity to pursue ambitious, fundamental research agendas that promise to define the future of computing and information.

4. Other interdisciplinary scientific computation related programs at the National Science Foundation, such as the *Cyber-enabled Discovery and Innovation* (CDI), *Cyberinfrastructure Training, Education, Advancement, and Mentoring for Our 21st Century Workforce* (CI-TEAM), *Grant Opportunities for Academic Liaison with Industry* (GOALI), *Software Infrastructure for Sustained Innovation* (SI2) etc.

5. Industry supported research centers, such as Nvidia's *CUDA Center of Excellence program*, Sony-Toshiba-IBM's *Center of Competence for the Cell Broadband Engine*, etc.

6. Industry supported research grants, such IBM's *Shared University Research* awards (SUR grants), Nvidia's *Academic Partnership Program*, AMD's *Fusion Fund Program* etc.

Finally, the Advisory Board of the Center will advise us in seeking funding from individuals and private foundations, and on forming industrial partnerships as a source of funds. These funds will take the form of donations to the Center, stipends for graduate and undergraduate students, and equipment.

2.6 Evaluation Measures

The effectiveness of the Center will be assessed by various factors, including the number of affiliates, external visitors, and publications, as well as the total amount of grant funds and private funds requested and obtained by Center affiliates.

3 Resources

The Center will have a strong initial cohort of affiliated faculty, with a significant and sustained record of grant funding and shared computational facilities. To support these existing strengths, the Center will require funding for a Director and an Associate Director, administrative and technical support staff, seed funding for Center affiliates, and graduate research assistants.

3.1 Faculty and staff

3.1.1 Faculty

The scientific computing group at UMass Dartmouth was formed by faculty members who wish to build on the common interests in their individual research programs to create a vibrant multidisciplinary and interdisciplinary group which can garner international recognition. These faculty members, many of them recent hires, have made scientific computing one of the core research competencies and potential signature research programs at UMass Dartmouth. The faculty members who will form the first cohort of Center affiliates are listed below.

Geoffrey Cowles (Assistant Professor in the Dept. of Fisheries Oceanography): Dr. Cowles' research is focused on the development and application of coastal ocean models. He has parallelized several codes including the popular open source unstructured-grid ocean model FVCOM which currently has 1500 registered users. Dr. Cowles implemented a parallel sparse matrix solve using PETSc to supply solution of the pressure Poisson equation in the non-hydrostatic version of FVCOM. Currently he is working on multigrid-based fully-implicit time-stepping schemes for ocean solvers and heuristics for mesh adaption in coupled hydro-sediment morphodynamic studies.

Yanlai Chen (Assistant Professor of Mathematics): Yanlai Chen received his B.S. degree in Mathematics from University of Science and Technology of China (USTC), in 2002, and Ph.D. in Mathematics from School of Mathematics, University of Minnesota, in 2007. Prof. Bernardo Cockburn was his thesis advisor. He then worked as a Postdoctoral Researcher supervised by Prof. Jan Hesthaven and Prof. Yvon Maday at Brown University. Dr. Chen joined Department of Mathematics, University of Massachusetts Dartmouth in August 2010, as an Assistant Professor in Mathematics. His research interests include the numerical solution of partial differential equations, including conservation laws and Hamilton-Jacobi-like equations and their applications. His expertise is in Adaptive numerical methods, especially the finite element discontinuous Galerkin Method, and reduced basis methods and reduced basis element methods.

Gary Davis (Professor of Mathematics): Gary Davis is Professor in the Department of Mathematics. He is former Boeing Distinguished Professor of Mathematics Education at Washington State University, and Professor of Mathematics Education at the University of Southampton, UK. He is currently carrying out research into successful mentoring of undergraduates in computational mathematics. He is working on establishing computational mathematics education as an identifiable branch of mathematics education, dealing with issues of computational experimentation, computational and statistical simulation in science

and mathematics, computational and statistical analysis including error analysis, and computational data analysis to promote high school and undergraduate interest in computational science. With many years of experience advising doctoral students he is also studying the process of mentoring graduate students in scientific computing.

Robert Fisher (Assistant Professor of Physics): The primary theme of Dr. Fisher's research is the fundamental physics of turbulent flows, and its application to the two endpoints of stellar evolution – star formation and supernovae – using a combination of theoretical and computational techniques. He is an expert in the field of astrophysical turbulence. While at Lawrence Livermore National Laboratory (LLNL), he developed the first quantitative theory of the distribution of stellar binary periods. As head of the astrophysics group at the Flash Center of the University of Chicago, Dr. Fisher led an international team of computational scientists and physicists in the development and analysis of the largest three-dimensional computer simulation of weakly-compressible fully-developed turbulence ever completed, on the massively parallel IBM Blue Gene/L (BG/L) machine at LLNL. Also at Chicago, Dr. Fisher was part of the team to carry out the first self-consistent simulation of the three-dimension detonation of a Type Ia supernovae. This research on turbulence and Type Ia supernovae was honored in 2009 by the DOE with a Certificate of Service. He is a primary architect of the Orion computational astrophysics code. His extensive experience in parallel algorithm development and scientific computing has included a wide range of numerical methods and platforms: ranging from the first generations of parallel machines, including the Connection Machine CM-5 and SGI Power Challenge Array to the most recent generations of massively parallel supercomputers, including the IBM BG/L and BG/P series.

Sigal Gottlieb (Professor of Mathematics): Dr. Gottlieb's overall research focus is the development of spatial and temporal methods for the efficient simulation of hyperbolic partial differential equations with shocks. She is internationally recognized as an expert on strong stability preserving (SSP) time discretizations, and has been funded by AFOSR since 2006 grant to develop SSP methods for the time evolution of hyperbolic partial differential equations, including problems requiring efficient and stable treatment of multi-scale phenomena. Dr. Gottlieb is also interested in post-processing for hyperbolic PDEs and spatial discretization methods for time-dependent PDEs, including spectral and WENO methods, as well as radial basis function methods.

Adam Hausknecht (Professor of Mathematics): Adam O. Hausknecht, who co-authored TEMATH with Prof. Kowalczyk, received his Ph.D. in algebra from U. C. Berkeley in 1975. In fall of 1982, he joined the Mathematics Department of the University of Massachusetts Dartmouth where he helped form the Department of Computer and Information Sciences (CIS). In 1996, he coauthored the graduate text Cogroups and Co-rings in Categories of Associative Rings with his thesis advisor, Prof. George M. Bergman, emeritus, U.C. Berkeley. He has taught a wide range of mathematics and computer science courses including calculus, differential equations, combinatorics, linear algebra, abstract algebra, category theory, integer programming, assembly language, C/C++, FORTRAN, Java, Pascal, Python, data structures, compiler design, computer graphics, and theory of computation. His interests include developing mathematics software for education, computer graphics, computer algebra systems, and noncommutative algebra. In fall of 2005, he resigned his joint-appointment with CIS and resumed a full-time appointment in the Depart-ment of Mathematics where he focuses on developing software for mathematics education, integrating software tools into the

mathematics curriculum, and scientific computation.

Alfa Heryudono (Assistant Professor of Mathematics): Dr. Heryudono's research focus is on numerical methods for PDEs based on RBF. He is currently developing adaptive local RBF method and its application to the simulation of human tear film. He is also working on RBF methods for time-dependent PDEs, in collaboration with Cheng wang, Sigal Gottlieb, and Saeja Kim from UMass Dartmouth, Jae-Hun Jung from SUNY Buffalo, and Scott Sarra from Marshall University. Dr. Heryudono is working with Elisabeth Larsson and Axel Målqvist from the division of scientific computing of Uppsala University in Sweden on a hybrid method finite element and RBF for problems in plate mechanics, for which they were recently awarded a Marie Curie FP7 agency grant beginning in May 2010.

Gaurav Khanna (Associate Professor of Physics): Dr. Khanna works on a variety of challenging problems in theoretical and computational physics. This primary research project is related to the coalescence of binary black hole systems using perturbation theory and estimation of the properties of the emitted gravitational radiation. This research is of relevance to the recently established NSF LIGO laboratory and the upcoming ESA/NASA LISA Mission that will attempt to make a direct observation of this radiation, and thus open a new window onto the Universe. Recently, Dr. Khanna has been an early explorer of the benefits of many-core architectures, such as GPUs and the STI Cell BE, and closely related software development frameworks like OpenCL, for scientific high-performance computing. Dr. Khanna obtained his Ph.D. degree from Penn State in August 2000 and his Bachelor of Technology degree from Indian Institute of Technology, Kanpur (India) in 1995. His research has been supported through grants from the National Science Foundation (NSF), private foundations and the computer industry.

Saeja Kim (Professor of Mathematics): Dr. Kim's research is focused on the areas of computational algebra, applied mathematics, and scientific computing. Recently she and her collaborators have published papers in the area of solid mechanics. She is currently carrying out research on edge detection, the development of post-processing methods, a numerical study of the effect of the parameter ϵ in WENO method, and a stability study of adaptive RBF simulations of convective flows, with her colleagues at UMass Dartmouth. Dr. Kim has been central to the NSF-funded CSUMS project where she serves as Director of Assessment and Student Research.

Steven Leon (Chancellor Professor of Mathematics): Professor Leon is Chancellor Professor in the Department of Mathematics at UMass Dartmouth. He is the author of Linear Algebra with Applications. It is one of the standard textbooks in linear algebra and is now in its 8th edition. It has been used by nearly every major university in the United States. International editions are widely used throughout the world. The book has been translated into five different languages. The book is known for its wide variety of applications and for its MATLAB based computer exercises. Professor Leon has been teaching linear algebra courses using computer projects for more than twenty years. He served as director of the ATLAST (Augmenting the Teaching of Linear Algebra using Software Tools) Project and has been a leading figure in promoting the use of computers in linear algebra courses and has played a major role in reforming of linear algebra education.

Mehdi Raessi (Assistant Professor of Mechanical Engineering): Dr. Raessi joined the Mechanical Engineering Department at UMass Dartmouth in 2010 following a postdoctoral study at Stanford University. He obtained his PhD in Mechanical Engineering from the University

of Toronto in 2008. He was then awarded a postdoctoral fellowship by the NASA/Stanford University's Center for Turbulence Research. Dr. Raessi's research focus is primarily on multiphase flows and free-surface flows with phase change. His research group develops and utilizes numerical models to study multiphase flows in various industrial and research applications including materials processing (spray coating), energy systems (fuel atomizers), "green" refrigeration systems, and submarine volcanic eruptions.

Nima Rahbar (Assistant Professor of Civil Engineering): Dr. Nima Rahbar received his B.Sc. degree in Civil Engineering from Sharif University of Technology, Tehran, Iran in 1998. He earned his M.Sc. in Civil Engineering in 2003 from Northeastern University and his Ph.D. in Civil Engineering from Princeton University in 2008. His doctoral dissertation was mainly focused on bioinspired design of functionally graded dental multilayers and interfacial fracture and adhesion in multilayered biomedical systems. Prior to joining the Department of Civil and Environmental Engineering at UMASS Dartmouth, he was a postdoctoral research associate at the Department of Mechanical and Aerospace Engineering at Princeton University.

Amit Tandon (Professor of Physics and Estuarine and Ocean Sciences): Dr. Tandon received his PhD. Mechanical Engineering, 1992, Cornell University. Dr. Tandon uses his knowledge of Fluid Mechanics and Physical Oceanography to address myriad of problems involving mixing processes in the upper ocean. He uses analytical and numerical modeling to address the importance of mixing and mixed layer processes for ocean circulation and climate. He has also supervised graduate students on basic experimental fluid mechanics projects. His research interests span from small- scale turbulence and oceanic mixed- layer processes, to sub-mesoscale frontal gradients and mesoscale eddies, and their role in setting up the large scale balances in the ocean.

Mazdak Tootkaboni (Assistant Professor of Civil Engineering): Dr Tootkabonis research lies at the intersection of computational mechanics and applied probability and statistics. He develops schemes that combine recent advances in stochastic modeling (e.g. stochastic PDE solving techniques) and applied statistics (e.g. machine learning and statistical inference) with the existing methods in computational mechanics. These schemes have a wide range of applications, from uncertainty modeling (representation and propagation) to model validation and from reliability analysis to integration of experiments and computational models, and fault tolerant (uncertainty informed) design topology optimization. He is an associate member of ASCE and a member of Engineering Mechanics Institute (EMI) and its Probabilistic Mechanics Committee.

Cheng Wang (Assistant Professor of Mathematics): Dr. Wang's primary research interest is the numerical solutions of nonlinear PDEs arising in natural sciences. He is currently focusing on the computation of incompressible fluid, including both 2-D and 3-D Navier-Stokes Equations (NSE), along with various models in Geophysical Fluid Dynamics (GFD). Both the collocation spectral method (jointly with Hans Johnston (UMass Amherst) and Jian-Guo Liu (Duke University)) and radial basis function (RBF) method (jointly with Sigal Gottlieb, Alfa Heryudono, Jae-Hun Jung and Saeja Kim at UMass Dartmouth) are taken into consideration.

Jay Wang (Associate Professor of Physics): Dr. Wang's research activities are in three related areas of atomic, molecular, and optical physics. The first one is to study the correlation effects in the interaction of light with matter. Dr. Wang uses a unique quantum perturbation method to calculate multi-electron transition cross sections in collisions of syn-

chrotron radiation with atoms such as helium and negative atomic hydrogen ions, and their interactions with nanostructures. Second activity relates to the interaction of strong laser pulses with Rydberg atoms. Dr. Wang calculates energy deposition, ionization and excitation cross sections, and quantum optical and nonlinear effects. His third major interest is in computational physics. His research involves numerically intensive work to model atomic and electronic processes occurring in reactions. He develops efficient computer codes using proven computational techniques in theoretical calculations.

3.1.2 Staff

For administrative support, the Center will require part-time $(20 - 25\%)$ secretarial support and also a similar level of support from a computer technician. The secretary will assist with the day-to-day operations of the Center (scheduling, handling seminar reimbursements, generating budget reports, etc.) while the technician will assist with the maintenance and upkeep of the Center's installed HPC hardware facilities.

3.1.3 Graduate research assistants

Graduate student support to enable collaborative research between the affiliates of the Center will be necessary for the initial few years. We expect that after two years, the Center will be able to support such students through (external) collaborative grant support.

3.1.4 Future positions

The Center may require additional administrative support in the long run. However such a position is likely not essential, initially.

3.2 Physical Facilities and Equipment

Office space. No specific physical space is required initially, since all the faculty are housed in their respective departments. However, in the future, having all the affiliated faculty in close proximity would clearly be beneficial.

Presentation and Meeting space. A multi-purpose space for meetings, presentations, graduate students, etc. would be highly beneficial to enable the activities of the Center. In addition, a digital visualization studio would enable Center affiliates to share the movies of their simulations with colleagues, and would provide a valuable resource for collaborative research and education endeavors.

Computing hardware. The group has several research-grade computation facilities to support the proposed Center: An 88-core traditional Linux compute cluster with 2.5 GHz Intel Xeon processors and 160GB of main memory; a novel 16-node compute cluster, built entirely from Sony PlayStation 3 (PS3) gaming consoles; IBM Blade Centers with 22 Cell Broadband Engine processors (9-core, 3.2 GHz) and 2 Power7 (8-core, 3 GHz) processors. Moreover, the group has just acquired a heterogeneous terascale parallel computer cluster incorporating graphics processing units (GPUs), which will become a shared campus research instrument. The many-core architecture of GPUs delivers a performance-to-cost ratio an order of magnitude higher than a conventional Beowulf cluster.

Data Center. With the natural growth of the scientific group and its future success will come more high performance computing equipment from new grants and start-up funds. We expect that within the next three years these computational equipment resources will outgrow the current data Center and will require housing at an off-campus location or significant renovations to the data Center. Alternatively, a different model for the Center's computational resource needs could be explored, based on the emerging paradigm of *cloud computing* i.e. the possibility of renting resources from a computing service such as Amazon's Elastic Compute Cloud.

3.3 Library/IT resources, materials, and supplies

3.4 Financing

The Center's financing plan will include Federal grant funding, industrial funding and partnerships, and private donations. There is also potential for additional funds through sale of consultancy services and research materials and technical reports.

3.4.1 Funding: Past, Present, and Pending

Members of the scientific computing group are currently funded by grants from the Office of Naval Research (ONR), Department of Energy (DOE), U.S. Air Force Office of Scientific Research (AFOSR), National Science Foundation (NSF), National Oceanic and Atmospheric Administration (NOAA), and various private foundations and industry. Together, they currently have more than $3M in grant funding on campus, and grant proposals for a total of $2.13M pending. Notably, the scientific computing group has recently been awarded two Federal grants which have enabled the acquisition of two heterogeneous terascale parallel computer clusters incorporating graphics processing units (GPUs). This state-of-the-art high performance computing instrument will serve as a a shared campus resource which will be used to develop the sophisticated, robust, and efficient GPU-accelerated high order algorithms for the large scale parallel simulation, postprocessing, and visualization of challenging problems including shock wave calculations, three dimensional turbulent flow, flows on complex domains with a high degree of localization, and simulation of star formation and gravitational waves. Furthermore, members of the scientific computing group have received NSF funding for a national conference to be held on campus on the topic of *Radial Basis Functions: Mathematical Developments and Applications*. This effort will draw national attention to the scientific computing group at UMass Dartmouth

Current grants: Members of the Scientific Computing group currently have approximately $3M in grants *on campus*, as well as participating in grants off-campus and bringing in funds to support students from exchange programs.

1. *An Investigation of Dynamical Processes Influencing Sediment Transport and Morphological Change in Skagit Bay using an Unstructured Grid Coastal Ocean Model.* ONR $115,000. PI: Cowles.

2. *An Assessment of the Tidal Kinetic Energy Resource off the Massachusetts Coast and Potential Impacts of Extraction.* MIT Sea Grant $150,000. PI: Cowles

3. *Modeling as a tool to better understand bay scallop recruitment and to manage bay scallop populations.* WHOI Sea Grant $150,000. PI: J. Churchill (WHOI), co-PI: Cowles.

4. *An Investigation of the Influence of Waves on Sediment Processes in Skagit Bay using an Unstructured Grid Model.* ONR $80,000. PI: Cowles.

5. *Effects of Tidal Power Generation on Sediment Transport in Muskeget Channel.* DOE $155,000. PI: J. Trowbridge (WHOI), co-PIs Cowles ($60,000), E. Terray (WHOI)

6. *MRI-R2 : Acquisition of a Heterogenous Terascale Shared Campus Computing Facility.* NSF $199,480. PI: Fisher, co-PIs: Cowles, Gottlieb, Khanna, Wang.

7. *A Heterogeneous Terascale Computing Cluster for the Development of GPU Optimized High Order Numerical Methods.* AFOSR (DURIP) $199,800. PI: Gottlieb, co-PIs: Fisher, Heryudono, Khanna, Kim, Wang.

8. *NSF/CBMS Regional Conference in the Mathematical Sciences-"Radial Basis Functions: Mathematical Developments and Applications.* NSF $35,000. PI: Kim, co-PIs: Gottlieb, Heryudono, Wang.

9. *High Order Strong Stability Preserving Time Discretizations for the Time Evolution of Hyperbolic Partial Differential Equations.* AFOSR $151,187. PI: Gottlieb.

10. *Positive Numerical Solution of ODEs.* KAUST $202,362.34. PI: Gottlieb.

11. *RUI: CSUMS: Research in Scientific Computing in Undergraduate Education (RESCUE).* NSF $ 469,969.00. PI: Gottlieb, co-PIs: Davis, Jung, Leon.

12. *FEM-RBF: A geometrically flexible, efficient numerical solution technique for partial differential equations with mixed regularity.* Marie Curie Research Executive Agency 117,397 Euro, at Uppsala University. PI: Elisabeth Larsson, co-PIs: Heryudono, Målqvist.

13. *GOALI: An Exploration of the Use of OpenCL for Numerical Modeling and Data Analysis.* NSF $166,499. PI: Khanna.

14. *Alternative Technologies for Numerical Relativity and Ligo Data-Analysis.* NSF $160,560. PI: Khanna.

15. *Summer Support of Graduate Student to Extend Scope of MS Thesis.* Foundational Questions Institute (FXQi) $3,750. PI: Khanna.

16. *Numerical simulations and analysis of the refrigeration system developed by Sunwell.* Sunwell Technologies Inc. $41,250. PI: Raessi

17. *GPU-accelerated numerical simulations of interfacial flows with applications in energy systems, material processing and bio-engineering.* Academic Partnership Program of NVIDIA Corporation, $3900 (Donation of a Tesla C2070 Graphical Processing Unit). PI: Raessi.

18. *Deposition of micro-particles and coating formation during the thermal spray coating process.* Rise Program of German Academic Exchange Service (Deutscher Akademischer Austausch Dienst) (DAAD): provides funding for one summer student. PI: Raessi.

19. *GPU-accelerated numerical simulations of multiphase flows with applications in energy systems and material processing.* Rise Program of DAAD: provides funding for one summer student. PI: Raessi.

20. *Interfacial Adhesion between Polymer Substrates and Osteoconductive Minerals - Addressing a Key Challenge in Bone Tissue Engineering.* University of Massachusetts Life Science Moment Fund $150,000. PI: Rahbar (with Jie Song).

21. *Submesoscale routes to lateral mixing in the ocean.* ONR $166,281. PI: Tandon

22. *On the importance of Submesoscale processes for ocean productivity.* NSF OCE $328,384. PI: Tandon

23. *Interpreting the oceans interior from surface data.* Subcontract from BU for a NASA grant $155,538. PI: Amala Mahadevan (BU), co-PIs: Tandon, Rob Scott (UT Austin).

Pending grants: Members of the scientific computing group have proposals out for $2.13M.

1. *CI-TEAM Demo: Portal of Powerful Cyber and Scientific Tools (POPCAST).* NSF $232,300. PI: Gary Davis, co-PIs: Erin Bromage, Robert Fisher, Sigal Gottlieb, and Alfa Heryudono.

2. *STCI : OpenCL for Scientific Computing.* NSF $646,668. PI: Fisher, co-PIs: Cowles, Gottlieb, Khanna, Raessi.

3. *Stability and adaptivity for reduced basis method and its applications to scattering problems with uncertainty.* NSF $309,157. PI: Chen

4. *Astrochemical Diagnostics of Turbulent, Magnetized Giant Molecular Clouds.* NSF $231,303. PI: Fisher

5. *COLLABORATIVE RESEARCH: Development of a robust pseudospectral-RBF hybrid method for fluid simulations with parameter reduction.* NSF $400,984.00. PI: Heryudono, co-PIs: Chen, Gottlieb, Kim.

6. *GOALI: Refactoring Numerical Relativity.* NSF $333,000. PI: Khanna.

7. *Investigating the dynamics of submarine volcanic eruptions using numerical simulations and laboratory experiments.* NSF $436,313. PI: Raessi, Co-PIs: Friedman, Tootkaboni, and Carey (URI).

8. *Submesoscale routes to lateral mixing in the ocean (Analysis Phase).* ONR $183,360. PI: Tandon.

9. *Multi-scale ocean modeling seamlessly integrated with mid-frequency acoustic simulators.* ONR $135,000 at UMass Dartmouth (of a total $7.5M). PI: Tandon, co-PIs: Fisher, Khanna.

10. *Collaborative Research: Stable and Efficient Convexity-splitting Schemes for Bistable Gradient PDEs.* NSF $104,283. PI: Wang (with Steven Wise of University of Tennessee).

Previous Grants at UMass Dartmouth: In the past decade, members of the scientific computing group have brought in over $1.5M.

1. Cowels' research was supported by grants from the WHOI and NOAA, totaling $196,000
2. Gottlieb's research was supported by grants from the NSF and AFOSR, totaling $345,718.
3. Khanna's research was supported with multiple grants from federal sources (NSF), private foundations (FQXi, Fund for Astrophysical Research, Glaser Trust of New York) and the computer industry (Apple, Sony, IBM) totaling to approximately $237,000.
4. Tandon's research was supported by grants from the ONR and NSF, totaling $812,965.
5. *SIAM Student Chapter Start up.* SIAM $400. PI: Heryudono, co-PIs: Wang, Higgs.

3.5 Budget Projection

Revenue stream The members of the Scientific Computing group have a current portfolio of external research and equipment funding totaling $3M, and this amount is expected to increase dramatically in the next few years due to the recent hires of active and productive faculty members, and the support and mentoring provided to them by the Center. We expect this amount to increase by $1M each year for the next three years. If we assume that these grants are typically three year grants, the projected amount of the indirect funds that will be brought into the University by this group is between $300K and $500K each year for the next three years. **The amount that the Center will see from these indirect costs will depend on the agreement between the Center and the Provost.**

In addition to the increased research grant funding brought in by faculty affiliates, the Center leadership will work intensively to obtain funding from Federal grants, Industry partnerships, and private foundations. We expect these efforts to result in funding of $200K per year for the first three years of the Center.

Expenditures Below is tabular summary of the annual projected budget for the Center's activities from University sources. We note that expenditures of the Center will, in some cases, save the University money by streamlining costs that are currently duplicated in several departments and colleges. Through the Center, University resources will be used more efficiently since they will be unified by function: the needs of scientific computing faculty are similar even though they are spread out in different departments. Furthermore, as indicated explicitly in the table below, many of the costs will be reduced or eliminated over time because they can be covered through successful Center research grants. In particular, over time we anticipate that the budget associated to the Graduate Assistantships, Travel, Consultants and Equipment will be eliminated or reduced to a minimum. The continuing costs from University sources will the support of the Director & Associate Director, Seed Funding for Center Faculty and a modest Travel budget for inviting external seminar speakers.

	Initial Base Budget	Annual Incremental Costs	
Expenditure Items	First Year 2011-2012	Second Year 2012-2013	Third Year 2013-2014
Director & Associate Director	$20,000	$20,000	$20,000
Seed Funds for Faculty	$50,000	$60,000	$70,000
Graduate Assistantships	$52,000	$26,000	-
Staff	20 – 25% (Secy. + Tech.)	20 – 25% (Secy. + Tech.)	20 – 25% (Secy. + Tech.)
Travel	$20,000	$15,000	$10,000
Consultants	$18,000	$9,000	-
Equipment and software	-	-	-

4 Organization and Bylaws

4.1 Organizational structure

The Center for Scientific Computing and Visualization at the University of Massachusetts Dartmouth consists of a Director and Associate Director, a Board of Directors comprised of the affiliates of the Center, an Executive Board, an external Advisory Board, and Research Assistants and Associates. The Director of the Center is appointed by and serves at the pleasure of the Chancellor of the University of Massachusetts Dartmouth. The initial appointment is for two years and is renewable subject to an evaluation of the Director's performance. The Provost or an appropriate Dean is the Director's immediate supervisor on all matters related directly to the operations of the Center. Figure 1 describes the hierarchy of the Center. The Center for Scientific Computing and Visualization shall operate according to its own bylaws and policies, in so much as these bylaws do not conflict with any official regulation, guideline or policy of the University of Massachusetts, nor with any provision of the Massachusetts General Laws.

4.2 Responsibilities

4.2.1 Duties of the Director

- To provide direction and leadership for the Centers scientific mission.
- To enhance the reputation of the Center by networking with well-known scientists around the world and publicizing the accomplishments of member of the Center.
- To appoint an an External Advisory board, and arrange virtual and in-person meetings with members of this board.
- To organize meetings, seminars, workshops and other activities that foster internal and external collaborations.
- To convene quarterly meetings of the Board of Directors and to preside over said meetings.

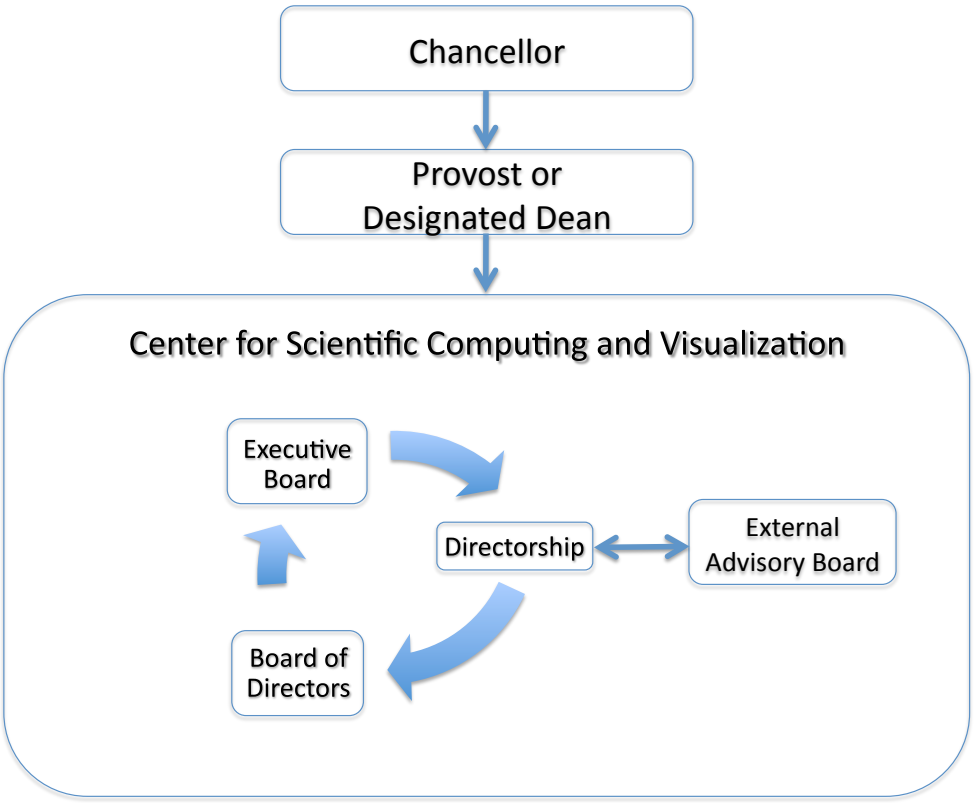

Figure 1: Hierarchy of the Center

- To convene quarterly meetings of the Executive Board and to preside over said meetings.
- To appoint new affiliates, subject to the approval of the Board of Directors.
- To appoint Research Associates and Assistants subject to the approval of the Board of Directors.
- To submit to the Executive Board a proposed annual budget
- To work with the Deans of the Colleges, and the appropriate Department Chairpersons on issues that pertain to affiliates of the Center.
- To submit an annual report in writing to the Board of Directors describing the Centers scientific activities.
- To submit an annual report in writing to the Provost and designated Dean describing the Centers activities, personnel, expenditures, and sources of funding
- To report to the designated Dean any changes to the Executive Board, Advisory Board, mission or bylaws.

- To advise and assist with graduate student recruitment strategies for the Computational Sciences track of the Engineering and Applied Science Doctoral Program.
- To maintain a record of research projects, publications, grant proposals, and current funding of all affiliates of the Center.

Evaluation of the Director The Director's performance of the duties described above will be evaluated by the Provost and designated Dean. Evaluation of faculty activities will be completed separately under the appropriate categories of evaluation established in the Agreement between the University of Massachusetts Board of Trustees and the University of Massachusetts Faculty Federation. The Director serves at the pleasure of the Chancellor and may be removed from this position by the Chancellor at any time. In addition, a Director may be removed before the expiration of his/her term of appointment by a two-thirds vote of the full Board of Directors, subject to the approval of the Chancellor of the University of Massachusetts Dartmouth.

4.2.2 Board of Directors

The purpose of the Center is to support and promote the affiliates interdisciplinary and multidisciplinary research in scientific computing. As such, the Board of Directors is the very heart and essence of the Center. The Board of directors will consist of all tenure-track and tenured faculty who are affiliates of the Center. They will advise the Director on setting the Scientific mission of the Center, and on the needs and objectives of each faculty member affiliated with the Center.

The initial Board of Directors will consist of the faculty members listed above. New affiliates will be eligible to join the Center at any time. Three members of the Board of Directors will be needed to nominate a new affiliate. In the nomination, they will state the qualifications of the candidate and the reasons for the appropriateness of the candidate to join the Center. A simple majority of the Board of Directors is necessary to recommend the new affiliate whose candidacy will be approved by the Director.

4.3 External Advisory Board

The purpose of the External Advisory Board is to connect the Center with the international scientific community. The Advisory Board shall be appointed by the Director in consultation with the Board of Directors. It shall be composed of individuals who are leaders in the field of Scientific Computing in its diverse manifestations. The Advisory Board shall assist in setting the Centers research agenda and in identifying opportunities for international collaborations and external funding. The Advisory Board are the ambassadors of the Center, promoting the work of the Center and establishing new associations with leaders in scientific computing.

4.3.1 Executive Board

The Executive Board will consist of the Director and Associate Director of the Center, two (2) members of the Board of Directors appointed by the Director, two (2) Center affiliates elected by the Board of Directors, and up to four (4) other individuals, whether affiliates of the Center or not, who are elected by the Board of Directors. Membership shall be for two (2) years and

renewable. All members of the Executive Board will sign an agreement to execute the mission of the Center in collaboration with other Executive Board members, and abide by the policy on Center operations. The Executive Board will be convened quarterly by the Director of the Center. Members will receive at least one week's notice prior to the quarterly meetings. A simple majority of the Executive Board shall constitute a quorum. A simple majority of those members present and voting shall be sufficient to grant or withhold the approval of the Executive Board on all matters, unless specified elsewhere in the mission statement and by-laws. Meetings will be run subject to Robert's Rules of Order. The designated Dean is an *ex officio* member of the executive board. The Provost and the Chancellor of the University of Massachusetts Dartmouth may attend any and all Executive Board Meetings.

1. The Executive Board will approve the External Advisory Board and any changes in its composition.

2. The Executive Board will be actively involved in the financial planning and administration of the Center.

3. The Executive Board will review the Director's quarterly update on research projects, service agreements, sponsored research agreements, and other activities.

4. The Executive Board will review the Director's quarterly statement of the budget for the Center and to make recommendations for expenditures and encumbrances from the budget.

5. The Executive Board will ratify or reject any changes, recommended by the Board of Directors, to the mission or bylaws of the Center, and to policies governing the Center's operations as specified in the mission statement and by-laws,

6. The Executive Board will approve or amend the Director's proposed annual report, financial statement, and proposed budget before it is submitted to the Provost or other officers of the University.

4.4 Bylaws

1. *Selection of Affiliates.* New affiliates may join at any time. A candidate will be nominated by three affiliates, voted on by the Board of Directors, and become a member subject to the approval of the Director.

2. *Responsibilities of Affiliates.* Affiliates of the Center will be committed to furthering the mission of the Center and supporting the research of other affiliates. Affiliates will note their affiliation with their Center on publications and in public lectures.

3. *Course Releases.* Affiliates of the Center who maintain an active research agenda will be assigned a teaching load of two courses per semester.

4. *Workshops and Seminars.* All workshops and seminars organized in collaboration with the Center will bear the name of the Center on all advertisements. All proceeds from registration for workshops will be placed in a revenue account administered by the Office of Research Administration, University of Massachusetts Dartmouth, for use by the Director to sustain growth within the Center.

5. *Website of the Center for Scientific Computing and Visualization.* All affiliates will have free access to the website of the Center and will be allowed to edit their section with no restrictions.

6. *Indirects costs from Grants.* **The Center will receive a percentage of the indirect funds generated by the grants of Center affiliates, to be determined**.

7. *Gifts to the Center.* All gifts will be placed in an endowment fund administered by the UMass Foundation, for use by the Director to sustain growth within the Center.

8. *Publications by Research Associates.* All scientific computing-related books, book chapters, and scholarly articles published by affiliates of the Center will note this affiliation. Any individual who receives financial or other resource support from the Center shall acknowledge or note the Centers assistance in any publications resulting from such support.

9. *Software, Curriculum and Related Professional Development Services.* Any software and education products produced by affiliates of the Center may be sold through the University of Massachusetts Dartmouth. Revenue collected from such ventures will be placed in a revenue account administered by the Office of Research Administration, University of Massachusetts Dartmouth, for use by the Director to sustain growth within the Center. In addition, such products and services can be provided by commercial partners through a legal licensing agreement or contract established by the Legal Counsel of the UMass Presidents Office.

10. *Travel Reimbursement.* All Center affiliates shall be eligible to receive supplemental funding for travel, subject to availability of funding, if approved by the Director, and subject to University policy. An individual shall ordinarily have exhausted all other sources of travel funding, including University entitlements, discretionary funding, and any grant funds allocated for travel before requesting funds from the Center. All papers presented at a scholarly or professional conference with travel assistance from the Center must include the individual's affiliation with the Center on the title page.

11. *Technical Reports.* The Center for Scientific Computing and Visualization will establish a series of technical reports, to be made available online. Any download fees associated with these technical reports will be set by the Board of Directors and approved by the Executive Board, and will be placed in a revenue account administered by the Office of Research Administration, University of Massachusetts Dartmouth, for use by the Director to sustain growth within the Center.

12. *Facilities Committee.* A Committee of three Center affiliates shall be appointed by the Director for the purpose of managing and maintaining existing Center facilities and also procurement. This committee shall meet at least twice annually to review the status of the Center's facilities.

13. *Technology Committee.* A Committee of three Center affiliates shall be appointed by the Director for the specialized purpose of managing and maintaining the Center's current HPC hardware and also planning and overseeing future hardware procurement.

This committee shall meet at least twice annually to review the status of the Center's compute hardware, and work with IT to plan for the future of HPC on campus.

14. *Library Committee.* A Committee of three Center affiliates shall be appointed by the Director for the purpose of collecting requests from the Board of Directors and recommending scholarly journals and other publications to the library. The Committee on Library and Acquisitions shall meet at least once annually to review the Centers library recommendation.

15. *Fundraising Committee.* A Committee of three Center affiliates shall be appointed by the Director with the main task of leading the Center's fundraising activities. This committee will target specific fundraising opportunities and will seek the assistance of all the Center's affiliates for this critical task. This committee shall meet at least quarterly and work closely with the Director and the Executive Board.

16. *Amendments and Changes to the By-Laws.* Any new by-laws or amendments to existing by-laws must be submitted in writing at a regular quarterly meeting of the Executive Board. All recommended amendments must pass a simple majority by the Board of Directors, ratified by a simple majority of the Executive Board and be forwarded by the Director to the Chancellor and Provost of the University of Massachusetts Dartmouth for approval.

5 Review and Assessment

The basis for evaluating the performance of the Center shall be

1. Success in securing external grants and contracts.

2. Success in producing scholarly publications in dissemination of research.

3. Success in engaging graduate students/postdocs in research.

4. Success in expanding faculty participation in interdisciplinary research.

5. Success in elevating UMD national/international impact in scientific computing research.

The activities of the Center will be reviewed every five years to ensure that it continues to serve its mission and the mission of the University. This assessment will include such objective measures as the total amount of grant funds and private funds obtained by the Center and the Center affiliates, and the number and quality of industrial partnerships and international collaborations, the number of affiliates and external collaborations established through Center activities, as well as subjective measures such as the satisfaction of the affiliates with the Center and the value they obtain from it.