University of Massachusetts Dartmouth
Center for
Scientific Computing and Visualization Research
2013 Annual Report

1 Overview

The Center for Scientific Computing and Visualization Research (CSCVR) at UMass Dartmouth unites a group 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. The impetus for the formation of the center came from the awareness of our significant multidisciplinary and interdisciplinary expertise in scientific computing, and the desire to leverage our existing strengths to build an internationally recognized center of excellence at UMass Dartmouth. The primary mission of the center is to transcend the traditional departmental boundaries and form a close-knit and collaborative multidisciplinary group who will combine wide range of mathematical, computational, and scientific skills to make significant impact across the field of computational science. The CSCVR's website can be accessed at cscvr.umassd.edu.

2 Review of 2013

2.1 Affiliates

CSCVR affiliates currently include more than twenty faculty researchers in mathematics, astrophysics, chemistry, biology, electrical and computer engineering, mechanical engineering, civil engineering, and the school of marine science and technology (see Appendix A). Our faculty publish in a variety of disciplines (see Appendix B for a list of 2013 publications), and are are funded by grants from the Office of Naval Research, Department of Energy, U.S. Air Force Office of Scientific Research, National Science Foundation, National Oceanic and Atmospheric Administration, and various private foundations and industry (see Appendix D for funding in 2013).

2.2 Scientific Advisory Board

One of our first objectives once the center was approved was to create a scientific advisory board comprised of leaders in the field of scientific computing and related sciences to assist in directing the the Centers research agenda, advise on research directions and trends in the field, and help identify appropriate collaboration and funding opportunities. We are honored and grateful that the following scientists have accepted to serve a three-year term as members of our scientific advisory board:
Marsha Berger, NYU, https://cs.nyu.edu/berger/
Jack Dongarra, University of Tennessee and Oak Ridge National Lab
http://www.eecs.utk.edu/people/faculty/dongarra/
Paul Fischer, Argonne National Lab, http://www.mcs.anl.gov/ fischer/
Ian Foster, Argonne National Lab, http://www.ci.anl.gov/people/profile.php?id=285
Antony Jameson, Stanford University, http://aero-comlab.stanford.edu/jameson/
Kirk Jordan, IBM, http://researcher.watson.ibm.com/researcher/view.php?person=us-kjordan
Randy LeVeque, University of Washington, http://faculty.washington.edu/rjl/
Robert Panoff, Shodor Foundation, http://www.shodor.org/about/board/panoff/
Stanley Osher, UCLA, http://www.math.ucla.edu/ sjo/

Richard Price, University of Texas, http://www.phys.utb.edu/ rprice/rprice.html
Chi-Wang Shu, Brown University, http://www.dam.brown.edu/people/shu/
Alex Pothen, Purdue University, Director of a DOE-funded Petascale Computing Group http://www.cs.purdue.edu/homes/apothen/

2.3 Activities

The CSCVR was officially created on January 10, 2013. In its first year, the center held one organizational meeting for the center affiliates, one research seminar day for the center affiliates, one open workshop that was open to all, and a series of faculty lunches.

Organizational Meeting: The organizational meeting focused on determining the most urgent needs of the CSCVR faculty and setting up committees that would support the work of the CSCVR. Some examples include a *computational facilities* committee to ensure the availability, maintenance and upkeep of the HPC cluster, a *library* committee to determine the most needed journals for center affiliates, reduce duplication of departmental requests for scientific computing journals, and inform the Dean of the Library of these needs, and a *fund raising committee* to look into funding opportunities both through scientific and infrastructure grants, opportunities from local industries, and other ways of funding the CSCVR's activities.

Research Seminar Day: In May we held a day-long series of 10-15 minute research presentations, to serve as an introduction of some newer faculty members (or newer research topics) and a springboard for collaborations. In addition to presentations by 14 faculty members, we had time for in-depth focused discussions in smaller groups.

Scientific Computing Workshop: In September we held two half-day workshops that consisted of research presentations by a number of CSCVR faculty and external visitors:

1. Yanlai Chen (Mathematics) spoke about reduced basis methods.
2. Mazdak Tootkaboni (Civil Engineering) discussed reducing offshore platform response to waves.
3. Akil Narayan (Mathematics) presented his work on blurring and de-blurring scientific models.
4. Vanni Bucci (Biology) introduced mathematical methods for assessing susceptibility and resistance to C. diff infection.
5. Mehdi Raessi (Mechanical Engineering) presented his computational simulations of energy systems.
6. Robert Fisher (Physics) spoke about exploding stars and the accelerating universe.
7. Bo Dong (Mathematics) Multiscale Simulations of Semiconductor Devices.
8. Firas Khatib (Computer Science) Crowdsourcing in the Computational Sciences.
9. Ying-Tsong Lin (WHOI) Underwater Sound Propagation.
10. Alfa Heryudono (Mathematics) Human Tear Film Dynamics.

Mentoring: A significant amount of time and effort was invested in the mentorship of new and junior faculty and researchers on matters associated to getting research programs off-the-ground, recruiting graduate students, seeking grant funding, and promotion and tenure requirements. These mentorship activities are at the heart of the activities of the CSCVR, as they promote our future success.

Computing Support: CSCVR associate director Gaurav Khanna has devoted much of his time to managing the HPC facilities and planning for future needs. He regularly meets with CSCVR affiliates as well as HPC hardware / software vendors in order to receive and review product updates and planning future acquisitions in order to stay competitive and continue to keep up with the growing computational needs of the CSCVR researchers. Moreover, our HPC facilities operate under consistently heavy load and require continued maintenance and repair, which Dr. Khanna has been providing.

2.4 Physical facilities

The center room renovation was completed in summer 2013 and provides an attractive and inviting work and collaboration space for faculty and students to congregate and has served as a catalyst for a number of new multidisciplinary projects.

The CSCVR facility has spaces for students and visitors to work and flexible collaboration spaces that can be used for seminars, large and small group meetings, lunches, and informal gatherings.

2.5 Computational facilities

The CSCVR has high performance computing facilities consisting of an IBM cluster with a total of 80 nodes (640 CPU cores), with 64 Nvidia Tesla GPU cards, networked with QDR Infiniband, and providing over 50 TB of NAS storage. This equipment was purchased in 2011 by two federal grants: an AFOSR DURIP grant and an NSF MRI award, as well as startup funds for new faculty members, Mehdi Raessi and Mazdak Tootkaboni. Our computational facilities reflect our emphasis on, and

expertise in, GPU computing. At last count, the computational facility now supports 20 faculty investigators and 28 postdoctoral, graduate student, and undergraduate student users. Additionally, it has been utilized in several undergraduate and graduate courses in the Mechanical Engineering, Mathematics, and Physics departments.

UMass Dartmouth pioneered the use of Sony PlayStation3s for astrophysics research back in 2007 when Gaurav Khanna of the Physics Department created a computer cluster of 16 PS3s and ran his black hole research simulations at supercomputer-level performance. These facilities were significantly augmented this year when the Air Force Research Lab (AFRL) at Rome, NY granted CSCVR four full racks (176 units) of Sony PlayStation 3s for research computing. This equipment transfer was under Dr. Gaurav Khanna's CRADA (AFRL) grant *Exploration of AFRL CONDOR for Scientific High-Performance Computation.*

In addition to our on-campus facilities, is invested in the Massachusetts Green High Performance Computing Center (MGHPCC), a data center dedicated to research computing that is operated by five of research-intensive universities in Massachusetts: Boston University, Harvard University, MIT, Northeastern University, and the University of Massachusetts. Our campus' contribution allowed us to buy in to the UMass system's HPC cluster and take advantage of additional significant computational resources. This system came online at the very end of 2013. Center actively participates in the governance and planning, user policy development and testing committees associated to the MGHPCC.

2.6 Education

The Center for Scientific Computing and Visualization Research promotes the mission of the University by providing undergraduate and graduate students with high quality discovery-based educational experiences that transcend the traditional boundaries of academic field or department.

CSCVR faculty are actively involved in mentoring undergraduate researchers and have been instrumental in preparing our undergraduate students for success in admission to high caliber graduate programs. Last year, Robert Fisher's students Kevin Jumper and Peter Jumper were admitted to prestigious graduate schools with fellowships. Kevin Jumper (B.S. Physics/Mathematics '13) worked with Dr. Fisher on numerical simulations of supernovae and is now a student at University of Texas Austin. His brother Peter Jumper (B.S. Physics/Mathematics '13) also worked with Dr. Fisher, on exploring the dearth of nearby Brown Dwarf companions to solar mass stars. Peter was an APS Apker Prize Finalist 2012, and declined the NSF Graduate Fellowship (2013), as well as Columbia University Dean's Fellowship (2013)

to attend the University of Toronto where he is funded under the Connaught Fellowship (2013). We are now starting to hear about our soon-to-graduate seniors Andrew Davey, Edward McClain, and Nicholas Moniz, who are being admitted to graduate programs and offered positions in industry. These will feature in next year's report. All these these students started their undergraduate research in the NSF-funded CSUMS program aiming to engage undergraduates in research in computational mathematics (see Appendix D).

Faculty in the CSCVR program have been working closely with students in the Physics masters' program, and this year Robert Fisher's student Suoqing Ji graduated and started a doctoral program in Physics at UC Santa Barbara. The CSCVR faculty were instrumental in establishing the "Computational Science and Engineering option in the newly created Engineering and Applied Sciences umbrella Ph.D. program at the UMass Dartmouth campus. The Center supports doctoral students in this track at various levels including: providing office space, computational resources, specialized coursework, access to a large team of computational researchers for advising and consultation, access to a variety of research projects, regular seminars series and in some cases, even fellowship funding. In the short 2 years that this program has been operating, CSCVR faculty currently support and supervise as many as 11 doctoral students that are working in very diverse research areas, from computational mathematics to oceanography, and even astrophysics! Many of these students have already passed the qualifying stage of the program and are progressing well towards doctoral candidacy. Several of these students have already started contributing to their research programs in the form of journal and conference publications. The number of doctoral students closely involved with the CSCVR are expected to grow dramatically over the next few years.

2.7 Research Highlights

To demonstrate the scope and breadth of the work being done by the CSCVR affiliates, we present a selection of recent research highlights of the scientific computing group:

- **Wave energy converters:** Sustainable energy extraction from ocean waves is a promising source of renewable energy, but the process of bringing a wave energy converter (WEC) design from the lab to commercial deployment is hindered by several critical scientific concerns that are difficult or impossible to study in the lab at early design stages of WECs. Computational methods can provide the ability to address such concerns early on in the development process and are capable of shortening the timeframe and associated costs of the design process. Mehdi Raessi (MNE), Mazdak Tootkaboni (CEN), and Geoff Cowles (SMAST) are developing an advanced computational tool foranalysis and optimizationofocean wave energy converters. This work was recently funded by the NSF with a grant of $368,221.

- **Black holes** It has often been suggested that a rapidly spinning black hole may capture a test particle (on a specifically designed trajectory) that would result in overspinning the hole, thus popping the horizon and forming a naked singularity in violation of the Hawking-Penrose Cosmic Censorship Conjecture. Gaurav Khanna (PHY) and collaborators have been able to numerically demonstrate the significant theoretical result that due to the effect of the conservative part of the gravitational self-force, this

overspinning simply does not occur.In other words, using high performance computing simulations, Gaurav Khanna (PHY) and his team were able to to explain why and how it is that a rapidly spinning black hole simply avoids capturing a test particle that could potentially overspin it!

- **Uncertainty quantification** Today's large-scale coupled systems are sensitive to various environmental perturbations, and mathematical modeling of such parametric variability through uncertainty quantification is required to ascertain failure rates of the system. Akil Narayan's (MTH) work focuses on adaptive and robust non-intrusive approximation methods for complex systems, with particular emphasis on computational techniques for high-dimensional uncertainty quantification. Mazdak Tootkaboni (CEN) is applying computational uncertainty quantification techniques and model validation for the design of thin-walled structures. His work develops a probabilistic paradigm for advancing analysis-based design. This work was recently funded by the NSF with a grant of $215,255.

- **Reduced basis methods** Many applications require simulations to be repeated tens of thousands of times to study the effect of the parameters on the solution. This repetition can be prohibitive in terms of computational time and cost. Reduced basis methods (RBM), are a model reduction framework that can provide a surrogate solution in negligible computational time based on pre-computed solutions. Yanlai Chen (MTH) is building a solid theoretical foundation for novel algorithm design to extend RBMs to a wider variety of problems including such real-world application areas as fine-tuning of the shape and material for stealth technology important to national security, design of solar cells for renewable energy, and non-destructive sensing. This work was recently funded by the NSF with a grant of $161,113.

- **Thermonuclear supernovae** The study thermonuclear supernovae has been recognized as critical for our understanding of the universe, as highlighted in 2011 when the Nobel Academy awarded the Nobel prize in physics "for the discovery of the accelerating expansion of the Universe through observations of distant [thermonuclear] supernovae." Of particular interest is the observation of highly unusual, subluminuous thermonuclear supernovae. If a standard brightness thermonuclear supernova can be thought of as a 60 watt light bulb, these subluminuous supernovae would be as faint as a candle. Robert Fisher (PHY), together with colleagues from the University of Chicago and the Weizmann Institute in Israel, has used high-performance supercomputer models of these supernovae to demonstrate that subluminuous events can be generated from explosions which fail to complete detonate the white dwarf star.

- **Time-stepping methods for integration of hyperbolic PDEs** Complex time-dependent fluid flows play a crucial role in a wide range of phenomena from the nanoscale to cosmic scales. The numerical simulation of these flows as they evolve in time is critical for the understanding of many important applications, and so the development of accurate and efficient time-stepping techniques is necessary across the sciences. Sigal Gottlieb (MTH) develops and analyzes numerical methods for time-evolution which are efficient and stable when used with a variety of spatial models.

Gottlieb and her team have recently created a numerical test suite that can be used by researchers to identify the best time-stepping method for specific simulations. This work has been funded by three grants from the AFOSR since 2006, with a recent award of $248,636.

2.8 Seminars and Visitors

- Seminar on January 30, 2013: Jan Tobochnik (Kalamazoo College) *Physical Insight From Computational Algorithms.*
- Seminar on January 31, 2013: Dalia Fishelov (Afeka–Tel-Aviv Academic College for Engineering) *Towards optimal convergence of a compact scheme for fourth-order differential equations with application to the Navier-Stokes system.*
- Seminar on February 5, 2013: Dana Fine (University of Massachusetts Dartmouth) *To infinity and beyond! (And back again): A rigorously-defined path integral for supersymmetric quantum mechanics and an easy proof of an index theorem.*
- Seminar on March 5, 2013: Mark Lyon (University of New Hampshire) *Fourier Continuation algorithms; fast transforms; and techniques for PDE Solution.*
- Seminar on April 9, 2013: Bernando Cockburn (University of Minnesota) *A short introduction to the devising of the HDG methods.*
- Seminar on April 16, 2013: Scott Field (University of Maryland) *Fast recovery of far-field signals from gravitational perturbations.*
- Seminar on April 23, 2013: Adrianna Gillman (Dartmouth College) *Fast direct solution techniques for elliptic partial differential equations.*
- Seminar on May 2, 2013: Mahadevan Ganesh (Colorado School of Mines) *Navier-Stokes equations on rotating surfaces: Regularity; algorithm; analysis; and simulation.*
- UMass Trustees James Buonomo and David Fubini visited the CSCVR on July 18, 2013.
- State Treasurer Steven Grossman visited the CSCVR on July 29, 2013.
- Seminar on September 18, 2013: Sergey Kushnarev (Singapore University of Technology and Design) *Geodesic equation on the Universal Teichmller space; Teichons; and Imaging.*
- Several colleagues from WHOI – Stace Beaulieu, Ying-Tsong Lin, and Arthur Newhall – joined us for the Scientific Computing workshops in September 2013.
- On September 29, 2013 the CSCVR hosted Georges Grinstein and Haim Levkowitz from the Institute for Visualization and Perception Research at UMass Lowell, Bob Haimes from MIT, and Nathaniel Whitaker from UMass Amherst for a meeting about extending simulation approaches to handling big data problems.

- Seminar on October 2, 2013: Jonny Zivku (Maplesoft) *Maple TA*,

- Seminar on October 17, 2013: Youssef Marzouk (Massachusetts Institute of Technology) *Tractable Bayesian computation for inverse problems.*

- On October 25, 2013 the CSCVR hosted the College of Engineering Dean's Advisory Board, consisting of:
  Ray Bellefeuille President of Phoenix Logistics, Inc.
  Kevin Brewer Executive Vice President Global Operations & CFO of Axcelis
  Bill Brum Section Head, Advanced Manufacturing Technology at Procter & Gamble Co., Inc.
  PierreCorriveau, Chief Technology Officer (CTO) at Naval Undersea Warfare Center (NUWC) Newport.
  David Marks, Goulder Professor Emeritus of Civil and Environmental Engineering and Engineering Systems MIT
  Norm Hildreth, Senior Vice President at Hittite Microwave
  Tom Jarbeau, Director and General Manager at Lockheed Martin Sippican, Inc.
  Michael Joyce, CEO of PrimaLoft, Inc.
  Teak Macedo, Managing Director at Phoenix Aerospace Consulting Group
  Carol Rego, Senior Vice President at CDM Smith, Inc.
  Chris Rezendes, President of Inex Advisors.
  Sanford Russell, Director of Marketing at GRID Business NVIDIA
  DaveSluter, CEO of New England Construction.
  Kevin Thibault, Vice President and Market Development Manager at Parsons.

- Seminar on November 6, 2013: Alex Lancaster (Harvard Medical School) *Rewiring robust yeast cellular networks: implications for evolution and human disease.*

- Seminar on November 12, 2013: Bob Panoff (The Shodor Education Foundation) *Parallel Thinking Across the Sciences: An introduction to computational thinking and modeling.*

- Seminar on November 13, 2013: Anil Zenginoglu (California Institute of Technology) *Infinity on a grid shell: solving hyperbolic equations on unbounded domains.*

- Seminar on November 20, 2013: Chris Poulin (Patterns and Predictions & The Durkheim Project) *Predicting the risk of suicide by analyzing the text of clinical notes and Distributed Machine Learning applied to Mental Health.*

- Seminar on December 3, 2013: Xiangxiong Zhang (Massachusetts Institute of Technology) *The asymptotic convergence rate of the Douglas Rachford iteration for basis pursuit.*

A Affiliates

Ramprasad Balasubramanian (Professor of Computer and Information Science): Dr. Ramprasad Balasubramanian received his PhD in Computer Science from the University of South Florida in 1999. He specializes in sparse- and large- data visualization methods, pattern recognition, computer vision, autonomous systems, mobile robotics and multi-vehicle autonomy. He has worked on several externally funded projects focusing on integration of wireless sensors into decision-making systems, sensor processing, sensor fusion and autonomous underwater vehicles. He is a member of IEEE, IEEE Computer Society and ACM. His work has been funded primarily by the Office of Naval Research (ONR) and the US Department of Transportation (USDoT)

John R. Buck (Professor of Electrical and Computer Engineering): Prof. Buck received his PhD from the MIT/WHOI Joint Program in Oceanographic Engineering in 1996. Prof. Buck's research focuses on signal processing, underwater acoustics and animal bioacoustics. His current funded projects investigate adaptive array processing, nonuniform spatial arrays, the design of active sonar waveforms, and the spatial information of animal biosonar. He also conducts research in engineering pedagogy. He is a Fellow of the Acoustical Society and a Senior Member of the IEEE. Dr. Buck is also received the IEEE Education Society Mac Van Valkenburg Early Career Teaching Award (2005) and the UMass Dartmouth Faculty Federation Teacher of the Year Award (2008)

Vanni Bucci (Assistant Professor of Biology) Dr. Bucci research interests lie in the integration of computational models and experimentation to study the dynamics of complex biological systems. Specifically, Dr. Bucci has worked in studying the ecological and evolutionary dynamics of multispecies microbial populations in environmental and engineered systems as well as those of human associated microbial communities in response to external perturbations.

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.

Bo Dong (Assistant Professor of Mathematics): Bo Dong received her 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. She held the position of Prager Assistant Professor of Applied Mathematics at Brown University for three years, after which she was a tenure-track assistant Professor at Drexel University. She joined our Mathematics Department in Fall 2012. Dr. Dongs research focuses on numerical methods for partial differential equations, particularly the analysis of the discontinuous Galerkin methods, hybridized Galerkin methods and mixed methods for second-order elliptic equations, transport equations, biharmonic equations and KdV type equations. In addition, Dr. Dong is developing a novel research program in the cutting-edge topic of multi-scale computations.

Lance Fiondella (Assistant Professor of ECE) Lance Fiondella joined the Department of Electrical and Computer Engineering in 2013. Prior to joining UMassD, he was a postdoctoral fellow in the School of Mathematical and Geospatial Sciences at the Royal Melbourne Institute of Technology (RMIT) in Australia. His PhD dissertation developed models to optimize the reliability of software based on its architecture. In addition to his reliability engineering research, he also participated in research at the Center for Resilient Transportation Infrastructure (CRTI), a Department of Homeland Security (DHS) National Transportation Security Center of Excellence (NTSCOE) at the University of Connecticut (UConn). He has published over 40 peer reviewed journal and conference papers. Four of his conference papers have been recognized with awards, including the 2011 best paper award from the International Conference on Reliability and Quality in Design (RQD) and the 2012 best paper award in the Attack and Disaster Preparation, Recovery and Response Track at the IEEE International Conference on Technologies for Homeland Security (HST). As a graduate student, he was the recipient of a National Science Foundation (NSF) East Asia and Pacific Summer Institutes (EAPSI) for U.S. Graduate Students, which enabled him to conduct collaborative research in the Department of Industrial Management at the National Taiwan University of Science and Technology (NTUST). He is a member of the IEEE Reliability Society and Vice-chair of Standard 1633, Recommended Practice on Software Reliability.

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 Department 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 Mlqvist 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. 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.

Firas Khatib (Assistant Professor in the Computer and Information Science Department): Dr. Khatib received his bachelor's degree in Applied Mathematics from UC Berkeley in 2001, and his Ph.D. in Bioinformatics from UC Santa Cruz in 2008. Dr. Khatib harnesses the collective brainpower of humans worldwide to tackle critical problems posed in computational biology. He worked with and studied how citizen scientists of the online protein folding video game Folditwith little or no prior biochemistry experienceuncovered knowledge that eluded scientists for years. He is interested in combining the power of humans and computers to tackle other difficult scientific problems. His research interests include bioinformatics, distributed computing, protein structure determination/prediction & design, machine learning, and molecular dynamics.

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 Emeritus of Mathematics): Professor Leon is Chancellor Professor Emeritus 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.

Maricris Mayes (Assistant Professor of Chemistry) joined the Department of Chemistry

and Biochemistry in January 2014. Dr. Mayes received her Ph.D. in Chemistry from Michigan State University in Fall of 2007. Prior to joining UMass Dartmouth, she was a postdoctoral fellow at Northwestern University and Argonne National Laboratory. Her research interest lies in the area theoretical and computational chemistry. In particular, she is interested in developing and applying highly accurate quantum chemistry methods for atomic, molecular, and biological systems. She has been involved in research efforts involving molecular and reaction dynamics, computational nanoscience, method/algorithmic development, and large-scale computing.

Akil Narayan (Assistant Professor of Mathematics): Dr. Narayan joined the Mathematics Department in 2012 following three years as a Visiting Assistant Professor at Purdue University. He holds a Ph.D. in Applied Mathematics from Brown University and works in the areas of numerical analysis, scientific computing, spectral methods, infinite intervals, and numerical solution of partial differential equations. His recent interests include Uncertainty Quantification.

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 Ph.D. 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.

Amit Tandon (Professor of Physics and Estuarine and Ocean Sciences): Dr. Tandon received his Ph.D. 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 (Associate 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 synchrotron 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.

B Publications in peer reviewed journals and proceedings

1. K. Adhikari, J. R. Buck and K. E. Wage, "Beamforming with Co-Prime Sensor Arrays," *Proceedings of the 2013 International Conference on Acoustics, Speech, and Signal Processing*, Vancouver, B.C., May 2013.

2. A. Amirzadeh,M. Raessi, and S. Chandra,"Producing molten metal droplets smaller than the nozzle diameter using a pneumatic drop-on-demand generator", Experimental Thermal and Fluid Science, Vol. 47, pp. 26-33 (2013).

3. A. Baskaran, J. Lowengrub, C. Wang, S. Wise, "Convergence analysis of a second order convex splitting scheme for the modified phase field crystal equation", SIAM Journal on Numerical Analysis, vol. 51 (5), 2013, 2851-2873.

4. A. Baskaran, Z. Hu, J. Lowengrub, C. Wang, S. Wise, P. Zhou, "Energy stable and efficient finite-difference nonlinear multi grid schemes for the modified phase field crystal equation", Journal of Computational Physics, vol. 250 (1), 2013, 270-292.

5. L. R. Berard,M. Raessi, M. T. Bauer, P. D. Friedman, and S. R. Codyer, "An investigation on the breakup of underwater buoyant oil jets: computational simulations and experiments, Atomization and Sprays" (in press - DOI:10.1615/AtomizSpr.2013007484).

6. L. M. Burko, G. Khanna, "Self-force gravitational waveforms for extreme and intermediate mass ratio inspirals. II: Importance of the second-order dissipative effect," Physical Review D 88, 024002 (2013)

7. W. Chen, C. Wang, X. Wang, S. Wise, "A linear iteration algorithm for energy stable second order scheme for a thin film model without slope selection", Journal of Scientific Computing, 2013, accepted.

8. Y. Chen, S. Gottlieb, "Reduced Collocation Methods: Reduced basis methods in the collocation framework." J. Sci. Comput. (2013) 55: 718 - 737.

9. Y. Chen, B. Cockburn, "Analysis of variable-degree HDG methods for Convection-Diffusion equations. Part II: Semimatching nonconforming meshes." Math. Comp. (2013).

10. Y. Chen, G. Davis, S. Gottlieb, A. Hausknecht, A. Heryudono, S. O. Kim, "Transformation of a Mathematics Departments Teaching and Research through a Focus on Computational Science", Journal of Computational Science Education, vol. 4, Issue 1, 24-29, Nov. 2013

11. S. Cooper, F. Khatib, D. Baker. "Increasing public involvement in structural biology." Structure, 21(9):1482-4 (2013) .

12. Cowles, G.W. , A Block-Structured adaptive mesh refinement solver for morphodynamic modeling Journal of Coastal Research, 29, 727-735 (2013).

13. A. Dubey, A. Calder, C. Daley, C. Graziani,R. Fisher, G.C. Jordan, D.Q. Lamb, L.B. Reid, D. M. Townsley, and K. Weide, Pragmatic Optimizations for Best Scientific Utilization of Large Supercomputers,International Journal of High Performance Computing, 27, 358, 2013.

14. M. Gargari, A. Louhghalam, M. Tootkaboni, "Optimal Cross Sections for Cold Formed Steel Members under Compression", Proceedings of 10th World Congress on Structural and Multidisciplinary Optimization, Orlando, FL, 2013.

15. Z. Guan, C. Wang, S. Wise, "A convergent convex splitting scheme for the periodic nonlocal Cahn-Hilliard equation", Numerische Mathematik, 2013, accepted.

16. Hakim, A., G.W. Cowles, and J.H. Churchill (2013), The Impact of Tidal Stream Turbines on Circulation and Sediment Transport in Muskeget Channel, MA. Journal of the Marine Technology Society, 47(4), 122-136.

17. J. Jakeman, A. Narayan, D. Xiu, "Minimal element stochastic collocation for uncertainty quantification of discontinuous functions", J. of Comp. Physics, 242:790-808, 2013.

18. S. Ji, R. Fisher, E. Garca-Berro, P. Tzeferacos, G. Jordan, D. Lee, P. Lorn-Aguilar, P. Cremer, and J. Behrends,The Post-Merger Magnetized Evolution of White Dwarf Binaries: The Double-Degenerate Channel of Sub-Chandrasekhar Type Ia Supernovae and the Formation of Magnetized White Dwarfs,Astrophysical Journal, 773, 136, 2013.

19. H. Johnston, C. Wang, J.-G. Liu, "A local pressure boundary condition spectral collocation scheme for the three-dimensional Navier-Stokes equations", Journal of Scientific Computing, 2013, accepted.

20. P. JumperandR. Fisher,Shaping the Brown Dwarf Desert : Constraints from Turbulent Fragmentation, Astrophysical Journal, 769, 9, 2013.

21. Gaurav Khanna: High-Precision Numerical Simulations on a CUDA GPU: Kerr Black Hole Tails, J. of Sci. Comp. 56, 366 (2013)

22. A. KumarandR. Fisher, The Astrochemical Evolution of Turbulent Giant Molecular Clouds: Physical Processes and Method of Solution for Hydrodynamic Starless Clouds, Monthly Notices of Royal Astronomical Society, 431, 455, 2013.

23. E. Larsson, E. Lehto, A. Heryudono, and B. Fornberg, Stable computation of differentiation matrices and scattered node stencils based on Gaussian Radial Basis Functions, SIAM Journal on Scientific Computing, Volume 35, Issue 4 (2013)

24. E. Larsson, S. Gomes, A. Heryudono, A. Safdari-Vaighani, Radial basis function methods in computational science. Reviewed and accepted for presentation and proceedings publication at the 13th International Conference on Computational and Mathematical Methods in Science and Engineering, CMMSE 2013. ISBN: 978-84- 616-2723-3

25. P. Manandhar, P. D. Calvert and J. R. Buck, "Elastomeric Ionic Hydrogel Sensor for Large Strains," IEEE Sensors, Vol. 12, No. 6, 2012, pp. 2056–2061.

26. A. Narayan, D. Xiu "Constructing nested nodal sets for multivariate polynomial interpolation" SIAM J. on Sci. Comp., 35:5, A2293A2315, 2013

27. R. H. Price, G. Khanna, Scott A. Hughes: Black hole binary inspiral and trajectory dominance, (in press) Phys. Rev. D (2013)

28. S. Ramachandran, A. Tandon and A. Mahadevan, "Effect of subgrid-scale mixing on the evolution of forced submesoscale instabilities", Ocean Modelling, Vol. 66, 45-63, (2013) http://dx.doi.org/10.1016/j.ocemod.2013.03.001

29. C. Rocha, A. Tandon, I. C. A. da Silveira, and J. A. M. Lima. "Traditional quasi-geostrophic modes and surface Quasi-geostrophic solutions in the Southwestern Atlantic". Journal of Geophysical Research: Oceans, (2013), DOI: 10.1002/jgrc.20214.

30. A. Taracchini, A. Buonanno, S. A. Hughes, G. Khanna: Modeling the horizon-absorbed gravitational flux for equatorial-circular orbits in Kerr spacetime, Phys. Rev. D 88, 044001 (2013)

31. M. Tootkaboni, A. Louhghalam, T. Igusa, "Statistical analysis of variability in floor response spectra using random vibration theory", Proceedings of the 11th International Conference on Structural Safety & Reliability, ICOSSAR, New York, NY, 2013.

32. K. E. Wage and J. R. Buck, "Snapshot performance of the Dominant Mode Rejection Beamformer," *IEEE Journal of Oceanic Engineering*, in press, DOI: 10.1109/JOE.2013.2251538.

33. K. E. Wage and J. R. Buck, "Convergence rate of the Dominant Mode Rejection beamformer for a single interferer," *Proceedings of the 2013 International Conference on Acoustics, Speech, and Signal Processing*, Vancouver, B.C., May 2013.

34. A. Zenginoglu, G. Khanna, L. M. Burko: Intermediate behavior of Kerr tails, (in press) Gen. Rel. Grav. (2013)

C Grants Submitted

Below we list the grants submitted in 2013 by faculty affiliates that listed the CSCVR to receive a portion of the indirect funds:

1. Bucci. *Collaborative Research: ABI Innovation: Predicting Multispecies Interactions.* Biology NSF $352,546.

2. Bucci, Chen, and Gottlieb. *Mathematics Modeling from Metagenomics.* Biology NIH $417,605.

3. Chen, Bucci, and Gottlieb. *Order Reduction Techniques for a Understanding of Gut Microbiota and Immune system function.* Math NSF $551,644.

4. Dong. *Development of Superconvergent Hybridizable Discontinous Galerkin Methods and Mixed Methods.* Math NSF submitted $252,248.

5. Gottlieb and Christlieb. *Numerical Methods for Long and Short Time Integration.* Math NSF $266,878.

6. Narayan. *Optimal High-Order Non-Intrusive Approximation Strategies for Plasma Physics Simulations.* Computational Math (YIP) AFOSR $346,586.

7. Wang. *Highly Efficient and Accurate Schemes for Nonlinear Gradient Flows.* Math NSF $268,798.

8. Khanna. *High-Precision (64-bit and higher) Floating-Point Operations using Hardware Single-Precision (32-bit) Operations.* DoD HPC PETTT Program $43,000.

9. Khanna. *Renewal: An Evaluation of Video-Gaming Technologies for Scientific High-Performance Computing in Gravitational Physics.* NSF CDS&E / PHY Program $90,000.

D Grants and Awards

Below we list the grants held in 2013 by faculty affiliates. These total over $5M.

1. John Buck, ONR *Co-prime Sensor Array Signal Processing*, 2013–2017, $743,000.

2. John Buck, ONR *Random Matrix Theory for Adaptive Beamforming*, 2012–2014, $404,000.

3. Yanlai Chen NSF award DMS-1216928, *Developing Reduced Basis Methods in the Galerkin and Collocation Framework*, 2012 –2015, $161,113.

4. Sigal Gottlieb, *Tailoring High Order Time Discretizations use with spatial discretizations of hyperbolic PDES*. AFOSR, 2012 – 2015, $248,633.

5. Sigal Gottlieb, Gary Davis, Steven Leon. *RUI: CSUMS: Research in Scientific Computing in Undergraduate Education (RESCUE)*. NSF 2009 –2013, $788,985.

6. Sigal Gottlieb, *Positive Numerical Solution of Differential Equations.* KAUST FIC grant, 2010 – 2013, $202,363.

7. Alfa Heryudono, *Development of a robust pseudospectral-RBF hybrid method for high-order moving interface simulation*, AFOSR 2013 – 2015, $40,000.

8. Gaurav Khanna, NSF *GOALI: An Exploration of the Use of OpenCL for Numerical Modeling and Data Analysis*, 2010 – 2014, $167,000.

9. Gaurav Khanna, NSF *Gravitation Theory: Numerical Modeling of Large Mass-Ratio Black Hole Binaries Using Time-Domain Perturbation Theory*, 2013 – 2015, $78,000.

10. Gaurav Khanna, Air Force *CRADA (AFRL): Exploration of AFRL CONDOR for Scientific High-Performance Computation*, 2010 – 2015, Equipment Share/Transfer.

11. Akil Narayan and Alfa Heryudono NSF *Computation of crowded geodesics on the universal Teichmuller space for planar shape matching in computer vision*, 2013–2016, $325,698.

12. Mehdi Raessi, Geoff Cowles, Mazdak Tootkaboni. NSF CBET *A comprehensive computational framework for analysis and optimization of wave energy converters*, 2012–2015, $368,221.

13. Mehdi Raessi, NSF CBET *Collaborative Research: Analysis and design of textured super-hydrophobic surfaces capable of preventing ice formation on wind turbine blades*,2013–2016, $214,583.

14. Amit Tandon, ONR *Submesoscale routes to lateral mixing in the ocean*, $349,641.

15. Amit Tandon, NSF *On the importance of submesoscale processes for ocean productivity*, $328,384.

16. Amit Tandon, NASA *Interpreting the oceans interior from surface data*, $129,318.

17. Amit Tandon, ONR *Coastal and Submesoscale Process Studies for ASIRI*, $647,173.

18. Mazdak Tootkaboni, *Collaborative Research: Uncertainty Quantification and Model Validation in Thin-Walled Structures: A Probabilistic Paradigm for Advancing Analysis-Based Design.* NSF $215,255

19. Cheng Wang, *Collaborative Research: Stable and Efficient Convexity-splitting Schemes for Bistable Gradient PDEs.* NSF 2011 – 2014, $104,283.

20. Yanlai Chen, Sigal Gottlieb and Adam Hausknecht were part of a group that was awarded a 2013-2014 Presidents Science and Technology Award from the UMass Presidents office ($150,000, awarded June 20, 2013).

21. Yanlai Chen, Bo Dong, and Vanni Bucci (from Biology) were awarded a Provost Seed grant for $31,000.