University of Massachusetts Dartmouth
Center for Scientific Computing
and Visualization Research
2014 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 that 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 `http://cscvr.umassd.edu`.

1.1   Affiliates

CSCVR affiliates currently include more than twenty faculty researchers in mathematics, physics, chemistry, biology, computer science, electrical and computer engineering, mechanical engineering, civil engineering, and the school of marine science and technology. Our faculty publish in a variety of disciplines, 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, Department of Defense, and various private foundations and industry.

New faculty: This year two new faculty joined UMass Dartmouth and became affiliates of the center. These faculty members do research in the field of data science and visualization: Dr. David Koop (Computer Science) and Dr. Donghui Yan (Mathematics).

David Koop received his Ph.D. from the SCI Institute of the University of Utah, and did his postdoctoral work at NYU. He is currently working on projects related to provenance, large-scale data analysis, and visualization. Dr. Koop served as one the core developers of the VisTrails project, where he led the development of a Provenance Software Development Kit that helps developers add provenance functionality to new and existing applications.

Donhui Yan received his Ph.D. in Statistics from the University of California- Berkeley, and was at Walmart Labs before coming to UMassD. His research interests are in Machine Learning, Applied Statistics, Data Science, and High Dimensional Statistical Inference.

1.2   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 CSCVR's research agenda, advise on research directions and trends in the field, and help identify appropriate collaboration and funding opportunities. Our current scientific advisory board consists of:

Mark Barnell, AFRL (Rome, NY)

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, UIUC, `http://mechanical.illinois.edu/directory/faculty/fischerp`

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/`

1.3 Computational Resources

Computational facilities *CPU/GPU cluster* 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.

Playstation cluster: 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 Barnell's group at the Air Force Research Lab (AFRL) at Rome, NY granted CSCVR nine full racks (396 units) of Sony PlayStation 3s for research computing. This equipment transfer was done under Dr. Gaurav Khanna's CRADA (AFRL) agreement.

MGHPCC: 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 the 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 totalling to over 10,000 processor-cores. This system came online at the very end of 2013. The center actively participates in the governance and planning, user policy development and testing committees associated to the MGHPCC.

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. Last year the advisory board recommended that we hire a professional technician. We have been working towards this, with various support models considered (including training graduate students and hiring them as part time technicians instead of teaching assistants!). Dean Peck has been advocating strongly for this, but to date this has not occurred and we have no information as to when and if this

will be possible. This is one of our main priorities for the coming year.

2   Review of 2014

In this review we highlight the changes that occurred in the past year, and the new activities undertaken this year. For background, please see the 2013 report.

2.1   UMass HPCday:

This year we initiated a UMass system-wide high performance computing (HPC) day conference. This one-day event highlighted the research in high performance computing (HPC) across the UMass system, at the Amherst, Boston, Dartmouth, Lowell, and Worcester campuses. At this event, we had ten speakers from across the system, in addition to Peter Tang from Intel and Kirk Jordan from IBM. Over lunch, Robert Panoff of the Shodor Organization gave a special presentation for students. The conference featured a poster session with over 30 presentations, and a student poster competition with prizes donated by SIAM and MathWorks. More than 100 attendees enjoyed the day of lectures and opportunities for collaborations. This conference was funded by UMass Dartmouth's vice-Chancellor for research Dr. Louis Goodman. Next year, we plan to expand this HPC day beyond the UMass system to include the other universities that are part of the Massachusetts Green High Performance Computing Center. We have already received $3,000 from the UMass President's office for next year's conference.

2.2   Major equipment donation to the CSCVR:

We recently received donations of two supercomputers that were built and used for mining Bitcoins. In December 2014, the New York Times covered Prof. Gaurav Khanna's novel use of PlayStations for his computational research in black hole astrophysics in a full length article. Two Bitcoin mining investors read the story and decided to donate their large supercomputers to the university campus for enabling research productivity further in the CSCVR. The two donated systems are very well suited to enable research in the CSCVR. The key feature of both systems is that they are GPU-accelerated, which makes these systems excellent for scientific applications of interest to the CSCVR faculty. The larger system amongst the two was built in 2012 at cost nearing a million dollars and consists of 180 servers installed in 10 racks, integrated tightly over a fast network.

The donor, Daniel Driscoll of San Francisco shares his thoughts on his donation: "This past winter during my morning commute, I stumbled across an article about a research project that recently used a networked super computer modeling the physics of black holes. Having grown up in the 80's next to the shuttle launch pad in Cape Canaveral, Florida, I remain an ardent fan of all things space. What struck me as even more interesting was how Professor Gaurav Khanna had created this super computer from now derelict Playstation 3 consoles. Being now part of the game industry, I was all too familiar with the transition of Playstation fans to the new flagship, the Playstation 4, and had myself done a few experiments to understand the potential uses for the no-doubt countless number of old Playstation 3's likely going to the trash. One such experiment involved a private venture to explore and understand the Bitcoin craze of 2013, a venture that ultimately proved fruitless but left me

in possession of not just several Playstations, but all also a large collection of what I had deemed a more effective array of server computers. Now that Bitcoin has come and gone for the hobbyist farmer, Professor Khanna and the University of Massachusetts Dartmouth has provided me an opportunity to join those explorers I once grew up with, if only in my own small way."

The donor of the smaller system chose to stay anonymous; we respect their privacy and therefore will not comment on any further details.

2.3   Notable Faculty Accomplishments:

- Ramprasad Balasubramanian was awarded a grant from the ONR on "Distributed Architecture to Address Communication Challenges in Achieving Multi-Unmanned Undersea Vehicle Autonomy"

- Vanni Bucci published a paper in Nature, on *Precision microbiome reconstitution restores bile acid mediated resistance to Clostridium difficile.* He was also awarded two new grants, one from the NIH on "Mathematical modeling from metagenomics - minimizing risk of enteric infections", and one from the NSF on "ABI innovation for predicting microbiome dynamics".

- Bo Dong was awarded an NSF grant for "Development of superconvergent hybridizable discontinuous Galerkin methods and mixed methods for Korteweg-de Vries type equations".

- Sigal Gottlieb was the opening plenary speaker at the International Conference on Spectral and High Order Methods (ICOSAHOM) in Utah, June 2014.

- Gaurav Khanna was awarded an NSF grant for "An Evaluation of Video-Gaming Technologies for Scientific High-Performance Computing in Gravitational Physics".

- Saeja Kim was awarded a AWM-NSF Travel Grant to attend the International Congress of Mathematicians (ICM 2014), Aug. 13-21, 2014, Seoul, Korea and the International Congress of Women Mathematicians (ICWM 2014), Aug. 12/14, 2014, Seoul Korea. At the ICM2014 conference she presented her work on "Symmetries and conservation integrals of nonlocal elastic fields" and her joint work with colleagues in the Department of Mathematics on Focus on computational mathematics as a vehicle for transformation of the educational experience, and its far reaching consequences at UMass Dartmouth. She also acted as section chair for a session on Mathematics Education and Popularization of Mathematics.

- Akil Narayan was awarded an AFOSR Young Investigator Program (YIP) grant for "Optimal and unstructured high-order non-intrusive approximations for uncertain parameterized simulations".

- Amit Tandon is one of two chief scientists for the U.S. Office of Naval Research Air-Sea Interactions in the Northern Indian Ocean Regional Initiative (ASIRI Departmental Research Initiative) collaboration with the Ocean Mixing and Monsoons (OMM) program of India supported by their Ministry of Earth Sciences. This involves bringing together the oceanographic community research PIs from about ten major US oceanographic research institutions and nine Indian research labs. and institutions. He also received a Fullbright Specialist Scholar award in July 2014, to visit the Indian Institute

of Science Bangalore. Dr. Tandon was awarded an NSF grant on "Collaborative Research: Role of mixed layer eddies on phytoplankton productivity in seasonally variable regimes" and an ONR grant on "Data serving for ASIRI participants".

- Mazdak Tootkaboni was awarded an NSF-CAREER award "CAREER: Predictive Analysis of Stability-Critical Structures: an Uncertainty-Informed Path from Measurements to Theory." He was also awarded a collaborative NSF grant for "Collaborative Research: Optimal Design of Flaw-tolerant Structures and Material Microarchitectures via Stochastic Topology Optimization."
- Cheng Wang was awarded an NSF grant for "Highly efficient and accurate numerical schemes for nonlinear gradient flows with energy stability".

2.4 In the News:

Based on a suggestion made by one CSCVR board member, we embarked on a PR campaign highlighting the successes of the center faculty and students. The main goal of this campaign was to raise campus-level and local community-level awarness of the center activities, on generate interest and support. We worked with the University's PR office and wrote several press-releases for dissemination within the campus community, and beyond. Some of these news stories were picked up by national media sources.

- Gaurav Khanna's use of playstations for astrophysics simulations, and of refrigerated shipping containers as housing for the cluster, was widely featured in a variety of news outlets, including the New York Times.
- An article about Sigal Gottlieb and scientific computing at UMass Dartmouth appeared in Bostinno.
- The UMassD website featured stories on CSCVR affiliates Gaurav Khanna and Sigal Gottlieb, and on our students Tiffany Ferreira and Sidafa Conde.
- The CSCVR room and affiliates were featured in several television ads for the UMass system.
- Our Playstation cluster has been the #1 in the RC5-72 cryptography challenge participant list for many months now. The RC5 challenge (Wikipedia) was originally started by RSA Laboratories as a worldwide contest to decode a cipher by finding the secret cryptographic key using a brute-force approach. The 72-bit version of the same contest continues today, conducted by distributed.net – one of the oldest open public distributed computing projects on the internet.

2.5 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. 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. There are currently 25 students in the entire EAS program, of whom 14 are in the CSE track and advised by center affiliates.

The CSCVR 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.

Student honors and awards

- Sidafa Conde has been named a 2014-2015 XSEDE scholar. XSEDE scholars are awarded support to hone research skills in high-performance and scientific computing. He was also invited to participate in the 2014 Brown-Kobe Joint Simulation School, and joined a group of students in this program for an exciting program in Providence, RI and in Kobe Japan. Sidafa was also awarded an SC14 Conference Broader Engagement (BE) Program Participation Grant on behalf of the SC14 General Conference Chair. Finally, Sidafa was recently selected for an internship at Sandia National Lab.

- EAS distinguished doctoral fellow Rahul Kashyap published his first peer-reviewed paper with Prof. Fisher in the leading journal Astrophysical Journal Letters, "Spiral Instability Can Drive Thermonuclear Explosions in Binary White Dwarf Mergers." Kashyap also presented a poster on this work at the international science meeting, "The Unquiet Universe," in Cefal, Sicily in June. At the same meeting, Prof. Fisher gave an invited presentation on work completed with Suoqing Ji (M.S. Physics '13), currently a Paxton Fellow in the Ph.D. program at the University of California at Santa Barbara.

- Zachary Grant presented a talk his work on "Strong stability preserving multi derivative methods" at a mini-symposium as part of the SIAM-CSE 2015 conference. He also presented a posted on "Strong stability preserving linear/nonlinear methods".

- Jiahua Jiang presented a poster on "Hybridized Reduced Basis Method and Generalized Polynomial Chaos for Solving Partial Differential Equations" at the SIAM-CSE 2015 conference. She also presented a poster on "Enhancements for Reduced Basis Methods: Reducing Offline Computational Costs" as part of an AWM workshop at the SIAM-CSE 2015 conference.

- Undergraduate student Jill Bolinger (B.S. Physics, '14) was just one of sixty students nationwide across all disciplines selected by the Council of Undergraduate Research to participate in their annual "Posters on the Hill" event in Washington, DC. In April, Jill had the opportunity to travel to Washington, DC to meet with members of the US Congress and Senate, and present a poster of her honors senior thesis research, conducted with Prof. Fisher, on the observational signatures of merging white dwarf binary supernovae.

- Three of our graduate students: Sidafa Conde, Zachary Grant, and Jiahua Jiang were awarded a SIAM travel award of $2,000 each to attend the 2015 ICIAM conference in China. Jiahua Jiang also received two AWM travel grants and two SIAM travel grants this year.

- Tyler Spilhaus and Jared Buckley published a conference paper titled "Parallel Performance of Higher-Order Methods on GPU Hardware" that appeared in the SpringSim/HPC 2015 conference at Virginia Tech.

- Rahul Kashyap published a paper in *Astrophysical Journal Letters* titled "Spiral Instability Can Drive Thermonuclear Explosions in Binary White Dwarf Mergers".

3 Summary

3.1 Current status

The ongoing budget constraints at UMass Dartmouth have been severe and have resulted in inadequate funding. The University has not yet established a budget for the CSCVR, and we have been currently operating through the generous support of the Dean of Engineering Robert Peck. He has advocated for us and provided us with funds from his own budget to cover the necessary basic needs. Our own funds, which are a portion of the indirect cost recovery from affiliate's grants, have started to be collected this year. We currently have approximately $11,000 in this account.

However, we have managed to accomplish much on these limited funds: first and foremost, we are providing mentoring of the junior faculty in research and grantsmanship and we are often told that this was a major contribution to their success in receiving grants, and to their general sense of well-being in their departments. Several faculty were awarded NSF grants this year, and we were very proud to have a NSF CAREER awardee and an AFOSR YIP awardee.

Second, the CSCVR has increased its visibility on and off campus, and its affiliates have been featured on the UMass Dartmouth front page and frequently in the Chancellor's *Monday Message* emails that are sent to the entire campus. We have also had local news articles published about the Playstation cluster and about the center, and now a New York Times article. These articles increased awareness of our strengths in high performance computing and prompted donations of new computational facilities to the CSCVR.

Thanks to associate director Gaurav Khanna and Dean Peck, we are also maintaining our current computational facilities, and planning for the future with the arrival of the new donated cluster, some needed upgrades to its memory, and other hardware needs.

3.2 Challenges and future plans

Last year the Scientific Advisory Board gave us very positive and constructive feedback on our activities and plans. One suggestion that was echoed by many board members was the hire of a computer technician. This has not yet been possible, but is one of our main priorities for the coming year.

A second suggestion by the board was to ensure that the University fund the center at the levels proposed when the center was approved. As mentioned above, the budget challenges have been severe, and we are hopeful that in the coming year this situation will resolve and we will be getting a budget. Our Provost, Dr. Mohammad Karim, has informed the campus that he expects cuts in next year's budget. However, the strategic plan just completed (UMASSDTRANSFORM2020) calls for prioritizing research activities and we hope that the new budget will reflect this focus despite planned cuts.

A third suggestion made by board members involved increasing our visibility both within the campus and outside. We have been able to do this well, and plan to continue this increased visibility in the coming year.

A caution sounded by several members of the board about the push toward engaging in "buzz-word" areas (such as big data). After much discussion individually with several members of the board, we felt that it may be beneficial to highlight the big data connection

in the work we do. It is important to continue to do the work that is meaningful to us while benefitting from the label "big data" and some of its approaches, as long as we are careful to stay focused on our primary area of interest.

Finally, board members suggested that we work to place talented students at National Labs for summer internships. We are pleased to report that Sidafa Conde has been accepted for a summer internship at Sandia National Lab.

There are two major projects that we are currently working toward: the first is a project that involves STEM eductions, and would allow us to bring Scientific Advisory Board member Dr. Richard Price to our campus in a formal capacity to develop new opportunities for undergraduate and graduate students in our programs. The second planned endeavor involves the Durkheim Project `http://www.durkheimproject.org/`. This project aims to use monitoring of social network user behavior to identify risk of suicide and enable intervention. It is an opt-in program that has been tested with active duty and veteran populations. We were approached by Chris Poulin, director and PI of this project, because he is well-aware that the CSCVR researchers have highly creative ideas and expertise in the area of computational science / big data analysis and could benefit from the research opportunities the project would bring. He is willing to move the project to UMassD if we help him implement it. This could potentially be an interesting opportunity for the CSCVR researchers to collobaroate with the social science departments on-campus.

Finally, in the fall we will be hosting the Finite Element Circus on our campus, with organizers Dr. Bo Dong and Dr. Yanlai Chen, `http://cscvr.umassd.edu/fec_fall2015/`