University of Massachusetts Dartmouth
Center for Scientific Computing and Visualization Research

Annual Report for July 1, 2019 – June 30, 2020

1 Goal and Mission

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 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. Our activities focus on creating a supportive and collaborative environment for computational science, and to support the computational needs of the CSCVR faculty and students. The CSCVR's website can be accessed at `http://cscvr.umassd.edu`.

2 Activities and Accomplishments

2.1 Major CSCVR endeavors

- **Fostering collaboration and mentorship of junior faculty and students.** A major component of our activities this year has been to support and mentor junior faculty. This year the CSCVR directors helped junior faculty members with editing grant proposals, tenure dossiers, etc. and also provided text on diversity, work environment, data management plans, and computational resources, to support proposal development.
- **Scientific computing throughout the disciplines.** The Center continued our new "lunchtime computing" series with a talks on the MIT *SuperCloud, Git & GitHub, Amazon SageMaker*. This series was suggested by our scientific advisory board and is being organized by Profs. Zheng Chen & Scott Field of the Mathematics Department.
- **Celebration of Director Gottlieb's SIAM Fellowship accomplishment.** On November 6th, 2019 the Center hosted an event to celebrate Director Gottlieb's SIAM Fellowship accomplishment. The event included remarks made by Center members, campus administrators, Dr. Chi-Wang Shu (Brown Univ.) on Director Gottlieb's impact on her department, the university and her field. This event was primarily organized by Drs. Yanlai Chen and Saeja Kim.
- **New collaboration with CVPA.** In Spring 2020, the Center began a new collaboration with the campus' College of Visual & Performing Arts. The underlying idea is for these two entities to interact at various levels, starting with curricula. As a test, a popular CVPA course on Virtual Reality (VR) was offered as a PHY (Physics), EAS (Engineering & Applied Science) and DSC (Data Science) elective. Unfortunately, due to the COVID crisis, the student experience in this VR class was severely hampered. This will need to be attempted again in the near future, under better conditions.

- **New cluster updates.** Our new DURIP funded cluster has been up and running since November 10, 2018. The cluster is currently in active use for the development and testing of innovative mathematical methods for applications that are of interest to the ONR, including wave-like phenomena, fluid transport, multi-phase flows and machine-learning based applications. To date, there are 68 user accounts (up from 41 last year) on the cluster. **As of June 29, 2020, the cluster has completed 422,890 jobs.** The new cluster is a factor of four more powerful than our old cluster. The new cluster has approximately 1,300 CPU-cores, 20 GPUs, 132TB storage, 3TB memory, with a peak compute performance of 180 TeraFLOPS and 2+ PetaFLOPS of machine-learning performance. The cluster has been used increasingly as faculty are porting their codes and starting to develop code on the new cluster. It is notable that the 15 nodes containing GPUs are used at a particularly high rate. This year the new clusters capability was enhanced by the installation of popular tools like *Matlab* and the *Jupyter notebook* environment. In addition, a dedicated Wiki was established that helps users get going on the cluster in a quick and efficient manner. The Wiki may be accessed here: `https://gitlab.com/cscvr/carnie-wiki/-/wikis/home`.
- **Leadership at the MGHPCC.** The Center continued to play a critical role in enabling major changes in governance and hardware architecture at the MGHPCC facility. Recall, that the Massachusetts Green High Performance Computing Center (MGHPCC) is a data center dedicated to research computing, operated by five of the research-intensive universities in Massachusetts: Boston University, Harvard University, MIT, Northeastern University, and the University of Massachusetts. This 5 year old facility provides race space and 15,000+ core cluster for use by UMass researchers. The Center Directors serve on the MGHPCC Research-Education-Outreach (REO) Committee and also the UMass system wide Faculty-Advisory-Committee (FAC) for the facility. Co-Director Khanna Chairs the latter, alongside another faculty member from UMass Amherst.

  One of the key efforts at the UMass system level this year was an increase in the investment in the context of Nvidia V100 GPUs. In particular, 2 high-end nodes, each with 4 V100 GPUs were purchased and installed in March.

2.2 CSCVR student and faculty accomplishments, prizes, and grant awards

2.2.1 Student and postdoc successes

By August 2020 we expect to graduate a very successful cohort of 4 EAS-CSE students including one going for postdoc at Brown University, and the other 3 in regional industry.

- Caroline Mallary (advisor Gaurav Khanna) defended her EAS doctoral thesis in July 2020 and will be a postdoc at ICERM, Brown University.
- CSCVR graduate student, Nur Rifat (advisors Scott Field & Gaurav Khanna) built and published a new computational model that aids in LIGO gravitational wave searches. Media stories on Nur's research may be found here:
  `https://www.umassd.edu/news/2020/umassd-graduate-student-aids-quest-understand-black-holes`
- CSCVR graduate student, Caroline Mallary (advisor Gaurav Khanna), was interviewed on a popular SciFi podcast about time-machines. Part 1: `https://www.podbean.com/ew/pb-srsei-db3205` and Part 2: `https://www.podbean.com/ew/pb-5578x-dc9f46`.
- Former student, Brian Pinault (advisor Robert Fisher) was recently hired as a public program specialist at Kitt Peak National Observatory.
- Dr. Fiondella's undergrad and grad students submitted a paper in a top-rated conference in the area of software reliability: J. Steakelum, J. Aubertine, K. Chen, V. Nagaraju, and L. Fion-

della, Multi-phase Algorithm Design for Stable and Efficient Model Fitting, Submitted to the International Symposium on Software Reliability Engineering, Coimbra, Portugal, 2020.

- Ben Burnett (advisor Maricris Mayes) completed summer internships at Los Alamos National Lab (summer 2019 & 2020).
- Michael Barquilla (advisor Maricris Mayes) completed a computational study of the effects of solvation of pyruvic acid (thanks to CSCVR summer fellowship).
- Graduate students Ardalan Nejat and his advisors Drs. Asadpoure and Tootkaboni have worked on computational strategies to address the challenge associated with the emergence of spurious modes in topology optimization with global stability considerations. This work was recently accepted for publication in Computer Methods in Applied Mechanics and Engineering journal.
- Graduate students Ardalan Nejat and Minhajur Rahman, supervised by Drs. Asadpoure and Tootkaboni, have accepted PhD positions at Johns Hopkins University and Case Western University, respectively.
- The graduate students Prosenjit Biswas, Rojin Ghandriz, and Osama Aljarrah from Dr. Jun Li's research group (Computational Mechanics and Materials Lab: `https://junli.sites.umassd.edu`) published five journal articles over the last year.
- In Fall 2020, EAS CSE alumna Jiahua Jiang will start a tenure track position at ShanghaiTech University, a new research university built in 2013 following the U.S. model and is in cooperation with several overseas schools such as University of California, Berkeley, University of Chicago, Massachusetts Institute of Technology, Drexel University, University of Padua and USC School of Cinematic Arts.
- Our former students continue to be successful in their careers. Dr. Sidafa Conde is a staff scientist at Sandia NM National Lab, Dr. Leah Isherwood is a staff scientist at Lincoln Lab, and Dr. Zachary Grant is a Householder fellow at Oak Ridge National Lab.

2.2.2 Faculty accomplishments and grants

- Research conducted in the CSCVR on black holes and the microbiome are among the papers published at UMass Dartmouth included in the 2018 Nature Index. The Nature Index, developed by the Nature Publishing Group, tracks research publications among a selection of 68 high-impact journals. These publications by CSCVR members accounted for nearly *half* of the total campus-wide high-impact publications over the past year.
- CSCVR faculty member Yanlai Chen (Mathematics) served as one of the lead organizers for a semester program on *Mathematics of Reduced Order Models* which had forty researchers in residence and three workshops which involved a combined total of over 300 researchers.
- CSCVR faculty members, Drs. Arghavan Louhghalam and Mazdak Tootkaboni (Civil & Environmental Engineering) were featured in *The New York Times* for their app that uses crowd-sourcing to measure and monitor the quality of roadways: `https://www.nytimes.com/2020/01/23/business/potholes-app.html`
- CSCVR faculty, Dr. Firas Khatib, gave an interview a computer game he co-developed, called "Foldit," that offers players the opportunity to search for cures of various diseases through protein building. Since then, more than 50 protein structures designed by the gamers. The full interview is available here: `https://pbn.com/five-questions-with-firas-khatib/`.
- CSCVR faculty, Dr. Robert Fisher's Computational Astrophysics Group was recently awarded a director's discretionary time allocation on the world's fastest supercomputer, *Summit*. Summit was developed by IBM and is operated by the Department of Energy Office of Science at Oak Ridge National Laboratory. This award will enable investigations of merging white dwarfs as a possible channel of Type Ia supernovae.

- Dr. Robert Fisher was part of an international team that recently published a research article in Nature that discovered how light reacts after a unique type of supernova. The team, consisting of researchers from Harvard University, Johns Hopkins University, Queen's University Belfast, University of Birmingham, University of Edinburgh, University of New South Wales, Trinity College Dublin, and the American Museum of Natural History and Space Telescope Science Institute found that light does not simply disappear after the cosmic explosion of stars.
- Dr. Fisher also published a paper jointly with observational colleagues in Nature Astronomy earlier this year, addressing the late-time light curves of Type Ia supernovae, one of his NASA ATP and NSF XSEDE awards. Another second paper written by CSCVR visitor Yossef Zenati, currently under review at Physical Review Letters, presents a new theory of universality and non-universality in a key process fundamental to astrophysical transients: turbulent nuclear burning.
- Co-Director Gaurav Khanna and his collaborators showed that nearly extreme black holes attempt to grow "hair", but ultimately fail! More about this new black hole phenomena can be found here:
  https://www.umassd.edu/news/2019/professor-discovers-way-differentiate-individual-black-hol
  html.
- Co-Director Gaurav Khanna's well-known work with Playstations received some attention again in *The Verge*: https://www.theverge.com/2019/12/3/20984028/playstation-supercomputer-ps3-umass-d
- Center Co-Director Gaurav Khanna was awarded a new research grant by NSF effective Sept 1st, 2020 - Aug 31st, 2022, titled "Studies of Black Hole Binary Systems Using Time-Domain Perturbation Theory".
- Drs. Geoff Cowles and Gaurav Khanna were awarded a new $100,000 MUST/ONR grant effective Feb 1st, 2020 - Jan 31, 2022, titled "Improving the Prediction Capability of Coastal Ocean Models Using Hardware".
- Dr. Arghavan Louhghalam was awarded the College of Engineering's inaugural "Equity, Diversity & Inclusion" award. The committee noted her initiative to design and participate in workshops to increase participation of junior high and high school girls in civil and structural engineering, her involvement in the society of women engineers, and leadership in an effort funded by the National Science Foundation to support panels and workshops on approaches to increase diversity and inclusion in the field of engineering mechanics.
- CSCVR faculty member, Leslie Chen, published one paper titled with "Multiscale convergence properties for spectral approximations of a model kinetic equation" in *Mathematics of Computation*, and another paper titled "A fast implicit solver for semiconductor models in one space dimension" is in press with the *Journal of Computational Physics*.
- Maricris Mayes is awarded a GHC Faculty Scholarship to attend the 2020 Virtual Grace Hopper Celebration.
- CSCVR faculty member, Maricris Mayes chaired a session at the 10th Triennial Congress of the International Society for Theoretical Chemical Physics, Tromso, Norway; together with her students, she also presented at national and international meetings.
- CSCVR faculty member, Maricris Mayes, received grant funding as Co-PI, from the ONR-MUST program for a project titled "Toward High-Power/High-Energy Flow Batteries for Applications in Unmanned Undersea Vehicles: Overcoming Fundamental Obstacles with a Bio-Inspired Active-Material Scaffold".
- Dr. Mehdi Raessi, Associate Professor of Mechanical Engineering, received a research grant and an REU supplement ($244K in total) from NSF for computational investigation of multiphase flow in the lung airway models, relevant to the surfactant replacement therapy in premature infants. Over the past year, he published three peer-reviewed journal papers with his students as the lead authors.

- CSCVR members Drs. Asadpoure and Tootkaboni and their collaborator have worked on an integrated element removal for minimum size and mesh sensitivity control in a discrete topology optimization framework. This work was published in Structural and Multidisciplinary Optimization journal.
- A doctoral student, Lijie Ji, of Shanghai JiaoTong University is visiting CSCVR faculty Yanlai Chen in the academic year 2019 – 2020 after secure a scholarship enabling her to visit any school.
- Multiple CSCVR faculty were awarded tenure and promotion: Drs. Maricris Mayes, Firas Khatib and Donghui Yan were awarded tenure and promotion to Associate Professor.

3   Total Revenue

Source	Amount
Indirect cost distribution	$30,716.84

4   Total Expenditures by Category

The Director's stipend and course release was funded from the College of Engineering budget. As the center did not receive its own budget allocation this year, we spent money infrequently. Our major source of funds was indirect cost distributions, which we have been saving up until we have sufficient funds for substantial needs. In the table below we report each of our expense this year:

Code	Expense detail	Amount	Description
PAY	Graduate student payroll	$25,491.25	Seed grants & student interns for summer
PAY	Payroll and fringe	$360.83	related to payroll above.
EX	Travel	$2,970.75	Seed Grants: student and faculty travel to conferences
AP	Conference Misc & Temp Space	$1,312.41	conference, seminars, and gatherings
AP	Educational Assistance	$5,327.22	Student tech. support
AP	Lab Supplies	$798.90	Oculus Rift & UPS battery backups
AP	Research Supplies	$2,000.01	
AP	Software	$20.00	For Dan Shao lab.
	Total Expenses	**$38,281.37**	

5   Employees and Consultants

5.1   Unofficial Staff

Although the center does not officially have any administrative assistants, Ms. Jill Peters (Math) and Ms. Anne-Marie Bedard (Engineering) have been very helpful to us. In particular, Ms. Bedard has assisted us with purchases for the CSCVR, and Ms. Peters with purchases and conference / event organization. In addition, Physics Dept. computer technician, Glenn Volkema, has been providing significant hardware support.

5.2   Internal Board of Center Affiliates

The CSCVR continues to grow as we have been hiring more faculty who have computational interests.
Alireza Asadpoure (Assistant Professor of Civil Engineering)
Ramprasad Balasubramanian (Professor of Computer and Information Science).
John R. Buck (Professor of Electrical and Computer Engineering)
Vanni Bucci (Assistant Professor of Bioengineering)
Geoffrey Cowles (Associate Professor in the Dept. of Fisheries Oceanography)
Yanlai Chen (Associate Professor of Mathematics)

Zheng (Leslie) Chen (Assistant Professor of Mathematics)
Joohyun Chung (Assistant Professor of Nursing)
Geoff Cowles (Associate Professor of Estuarine and Ocean Sciences)
Gary Davis (Professor of Mathematics)
Bo Dong (Associate Professor of Mathematics)
Scott Field (Assistant Professor of Mathematics)
Dana Fine (Professor of Mathematics)
Lance Fiondella (Associate Professor of ECE)
Robert Fisher (Associate Professor of Physics)
Sigal Gottlieb (Chancellor Professor of Mathematics)
Adam Hausknecht (Professor of Mathematics)
Alfa Heryudono (Associate Professor of Mathematics)
Gaurav Khanna (Professor of Physics)
Firas Khatib (Assistant Professor in the Computer and Information Science Department)
Saeja Kim (Professor of Mathematics)
Steven Leon (Chancellor Professor Emeritus of Mathematics)
Jun Li (Assistant Professor of Mechanical Engineering)
Arghavan Louhghalam (Assistant Professor of Civil Engineering)
Maricris Mayes (Assistant Professor of Chemistry)
Mehdi Raessi (Associate Professor of Mechanical Engineering)
Ming Daniel Shao (Assistant Professor of Computer and Information Science)
Amit Tandon (Professor of Mechanical Engineering and Estuarine and Ocean Sciences)
Mazdak Tootkaboni (Associate Professor of Civil Engineering)
Cheng Wang (Associate Professor of Mathematics)
Jay Wang (Associate Professor of Physics)
Donghui Yan (Assistant Professor of Mathematics)

5.3   External 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/`

6 Physical Space Occupied

6.1 Physical facilities

The center facility is in the Textiles building room 105 (TXT105). 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. The computer clusters belonging to the CSCVR are housed in the data center, and in a refrigerated container with a new mural designed by a Physics undergraduate.

6.2 Computational Resources

Microway CPU/GPU cluster The primary CSCVR has high performance computing facilities consisting of a HPC cluster with a total of 52 nodes (1,300 CPU cores), with 20 Nvidia Volta GPU cards, networked with EDR Infiniband, and providing over 130 TB of ZFS storage. This equipment was purchased in 2018 by an ONR DURIP award led by Director Gottlieb. Our computational facilities reflect our emphasis on, and expertise in, GPU computing. At last count, the computational facility now supports 40+ faculty investigators, graduate and undergraduate student users. The cluster has completed over 400,000 separate compute jobs since its installation.

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 3 years ago when Dr. 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 Gaurav Khanna's CRADA (AFRL) agreement.

ARNiE: In 2015 we received donations of two supercomputers in response to the New York Times article on Prof. Gaurav Khanna's novel use of PlayStations for his computational research in black hole astrophysics. 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 over a gigabit network. This cluster (called ARNiE, after our campus' mascot) nodes have 8-core Intel Core i7 CPUs, an Nvidia CUDA "Fermi" GPU and 24

GB of main memory. The cluster also has 130 TB of attached (available) storage that was recently upgraded to 200 TB.

Elroy: The CSCVR recently debuted a new innovative prototype supercomputer built entirely of mobile-devices (in particular, Nvidia Tegra X1 components used to build tablets) dubbed "Elroy". The system's total raw compute capacity is 16 teraflop/s and consumes just over 300W total power. The unique feature of this 32-node system is its extremely high power efficiency – an order-of-magnitude larger than traditional systems. This was made possible by leveraging recent, very significant power-efficiency related advances that have been cleverly engineered into current cell phones and other mobile devices (to prolong battery life). Power-efficiency is a limiting factor in large scale supercomputing as well, due to the expenses associated to large power consumption and corresponding cooling requirements. Elroy demonstrates a unique approach towards potentially meeting this challenge. This project was a result of a collaborative effort between the CSCVR and UMass Dartmouth CITS.

Rapid Prototyping Server I & II: Rapid prototyping servers (RPS1, RPS2) are high-end Linux servers with dual 3.2 GHz multicore Xeon CPUs, 256GB RAM, and a single high-end CUDA GPU each. Popular rapid prototyping software such as Anaconda Python 2 and 3, Julia, MATLAB with parallel computing toolbox, and Mathematica with GPU support were also installed. With convenient feature such as UMassD logon, the server can also be seen as an extension of faculty's office workstations or as a test machine prior to scaling up computing jobs to UMass Dartmouth multinode servers: ARNiE and HPCC or MGHPCC (UMass-wide supercomputer). Prototyping projects currently conducted on these machines include, but not limited to, deep learning with Mathematica, numerical simulation of systems of PDEs, development of new time-stepping methods, and preconditioning techniques for generalized finite difference sparse systems.

HPE SwitchBlade: Through a combination of a HPE "SwitchBlade" grant and start-up funds from two new faculty (Asadpoure and Louhghalam), the CSCVR installed a 8-node blade system with a total of 320 cores and nearly half a TB of main memory. The system will be used to support of the research of the new faculty and also explore virtualization in HPC.

MGHPCC: The University of Massachusetts system acquired a shared HPC cluster, which came online at the very end of 2013 that currently sports over 15,000 processing CPU cores and a large mount of memory. This cluster is installed at the MGHPCC. Unfortunately, this cluster was designed primarily for scientists in the life sciences, and CSCVR affiliates have found that their codes scale poorly on these machines, and in fact are faster on our old local machine by a factor of 10 (and if our GPUs are included, a factor of 100). Over the past two years, several of these issues were addressed. CSCVR Directors continue to work closely with the UMass Dartmouth administration and the UMass President's office to advocate for the needs of the CSCVR researchers.

Visualization equipment: In addition to the two 80" Sharp touchscreen displays, the center also procured and installed an interactive Panasonic 3D TV and an Oculus Rift VR system.

7 Projected Budget and Goals for Coming Year

In the past we requested funding for the CSCVR to support over thirty faculty affiliates and close to thirty students and postdoctoral researchers. This funding was not given. Since last year it became clear that beyond the director stipend and course releases, the CSCVR is expected to support itself using the indirect funds allocation from the affiliates' grants.

We have managed to accomplish much on these limited funds: first and foremost, we are providing close 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, retention and to their general sense of well-being in their departments. CSCVR affiliates are among the most successful researchers on campus, as evidenced by innovative publications and success in attaining grant funding. Second, the CSCVR has increased its visibility on and off campus, resulting in increased awareness of our strengths in high performance computing and attracting significant donations of hardware. We have created an identity as a center of multidisciplinary scientific computing that is now recognized nationally. This has greatly benefited us in attracting new hires.

7.1   Proposed Budget for 2019–2020

Director's Stipend	$15,000
Course buyouts (1 per semester)	$15,000
CSCVR Student Tech Support	$20,000
CSCVR Fellowship (one doctoral student)	$20,000
Seed funding for CSCVR affiliates	$20,000
Computational needs	$8,000
Total	**$98,000**

7.2   Goals

The following are our priorities for the coming year:

- Continue to increase our visibility both within the campus and outside, through seminars and conferences.

- Create and maintain mentoring and collaboration opportunities for center affiliates, through regular seminars, workshops, lunches, and other informal events (picnics), as well as meeting with junior faculty to create mentoring relationships.

- Maintain and upgrade our computational facilities. Thanks to Co-Director Gaurav Khanna and Dean VanderGheynst we are maintaining our current computational facilities. We are also working with the CIO Holger Dippel and Andrew Darling to ensure that the university Data Center be regularly updated to ensure stability of our electrical and cooling system.