



iACS

INSTITUTE FOR ADVANCED
COMPUTATIONAL SCIENCE

ANNUAL REPORT 2016

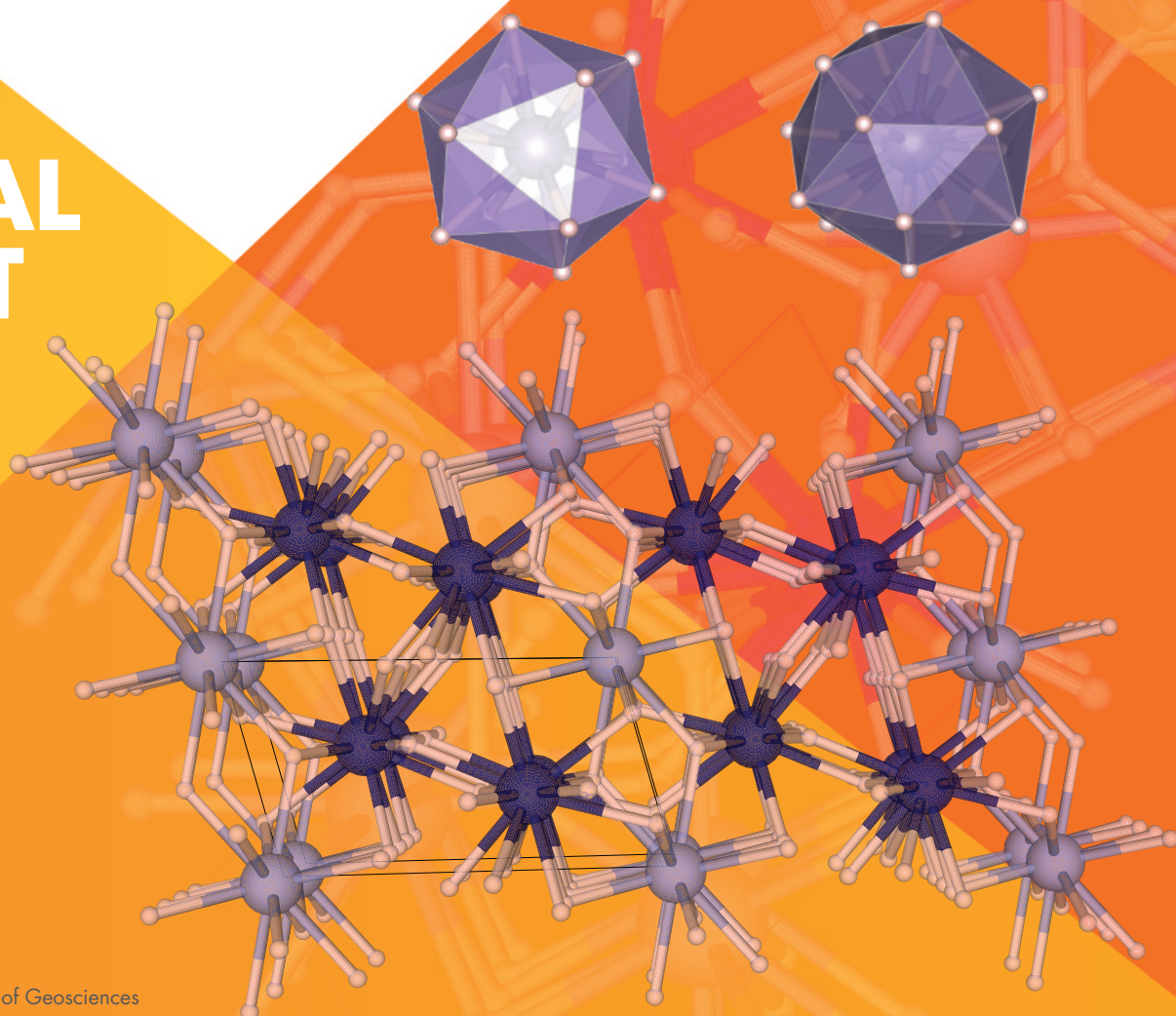


Image by Mahdi Davari, Department of Geosciences
Superconducting germanium hydrides

MESSAGE FROM THE IACS LEADERSHIP TEAM

Alan, Lynn and I are delighted to share with you this annual report that describes some of the exciting IACS events and accomplishments from the past year, and highlights our new colleagues.

We are delighted to have been awarded a five-year \$3M National Science Foundation Research Traineeship (NRT) grant to prepare the next generation of scientists working with big data to support complex decision-making (STRIDE – Science Training & Research to Inform DEcisions). Our highly interdisciplinary team spans the departments of Applied Mathematics and Statistics (AMS), Biomedical Informatics, Computer Science (CS), Ecology and Evolution, and the schools of Journalism and Marine and Atmospheric Sciences (SoMAS), and includes external partners such as IBM and Brookhaven National Laboratory where students will go for internships. STRIDE will include a new advanced graduate certificate that is in the final stages of internal approval at Stony Brook.

Speaking of graduate certificates, the first courses for what will be CDCSE (Certificate in Data and Computing for Scientists and Engineers) are now being offered. The certificate is another wonderful illustration of the multidisciplinary spirit and plans of IACS, and presently serves all of SBU with 96 courses from many departments including Physics, AMS, SoMAS, Sociology, CS, and Materials Science & Engineering (with others poised to be added).

SeaWulf, the new high-performance computer supported by a \$1.4M grant to IACS from the National Science Foundation with \$0.6M match from NYS and internal SBU sources, is now fully operational and is freely available to everyone across campus. We recognize the huge effort required to do this by our HPC system administrators (Firat Coskun and Eric Rosenberg) and other staff from the Division of Information Technology (DoIT). The new cluster nearly triples the open computing resources on campus and, to emphasize that openness, is being shared through the new DoIT Research Computing organization.

Our pursuit of external funding continued this year with 16 proposals submitted for a total of \$9,540,582: two proposals are still pending (valued at \$948,341) and nine were awarded (valued at \$4,992,331).


We would like to highlight just two of the many events held in the last year. In conjunction with the Center for Inclusive Education (CIE), we hosted Prof. Richard Tapia, a national leader in diversity in the mathematical/computational sciences and director of the Center for Excellence and Equity in Education at Rice University. As part of his visit we held “Drawing Diversity to Academia,” a panel session designed to discuss opportunities, best practices, and novel ideas for increasing the participation and success of underrepresented minorities in the STEM fields. Distinguished panel members included Prof. Tapia, Noel Blackburn (BNL), Dr. Frances Brisbane (SBU), Dr. Dennis Assanis (SBU); Dr. Carlos Medina (SUNY), Dr. Charles Robbins (SBU), Toni Sperzel (SBU), and Dr. Charles Taber (SBU). Last summer we also held the second “IACS Computes!” summer camp for local high school students, an immersive 10-day workshop that uses a project-based approach and the Python programming language to introduce students to the programming skills and software/computer technologies that drive advances in science, industry, business, and society. The materials from this event subsequently enabled us to construct teaching materials that were shared by us in training sessions that spanned two weekends with regional master teachers to form the basis of their new curricula.

Multiple new faces joined us this year, bringing new perspectives and fresh energy to IACS. Professor Jeffrey Heinz will be joining IACS as a core faculty member in the fall of 2017 from the Department of Linguistics and Cognitive Science at the University of Delaware. Eric Rosenberg started with IACS in July of 2016 as a Senior HPC Engineer to help manage our on-campus computing clusters and is jointly supported by DoIT. Professor Hideo Sekino comes to IACS from the Toyohashi University of Technology in Japan as a part-time Research Professor working with Harrison. Dr. Tony Curtis is a new Programming Project Leader, working with Professor Barbara Chapman’s group. Rosalia Davi joined IACS in March 2016 as the Diversity Outreach Coordinator jointly supported with CIE to pursue our shared objectives in diversity and broad participation. In addition we have 4 new faculty affiliates from Ecology & Evolution, SoMAS, Neurobiology & Behavior, and the School of Journalism. We also draw your attention to our graduate student awards on page 20 for Aditii Ghai, Philip McDowell, Eric Raut, Adrián Soto and Zeyang Ye.

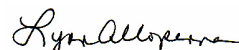
IACS is very grateful to many people, especially our generous endowers and the SBU university leadership, specifically President Stanley, our new Provost Bernstein, Vice President of Research Reeder, Dean Kopp, and Dean Sotiropoulos who have all been steadfast in their support of our events, strategic and opportunity hires, and overall mission. We are also immensely grateful for the continued support and shared vision of the faculty and department chairs of all of our partner departments, and from Brookhaven National Laboratory notably including Deputy Director Robert Tribble and Director of the Computational Science Initiative Kerstin Kleese van Dam.

This year we would like to give special thanks to Assistant Dean for Diversity & Inclusion and Director of CIE Toni Sperzel for her tireless efforts in helping us work to increase and support diversity in our ranks and her support for STRIDE; Chief Information Officer Melissa Woo for her leadership and investments in establishing research computing at Stony Brook as well as the efforts of her staff including Sanjay Kapur and the HPC system administration team recognized above; Laura Lamonica who keeps IACS so bright and shiny, and whose dedication and good cheer are not daunted even by the worst blizzard; Rosalia Davi, Prof. Marivi Fernández-Serra, and Adrián Soto for so successfully representing IACS at the Tapia and Hopper conferences (see pages 12-13); to Amilios Sofianopoulos, president of the IACS Student Association, for the energy and enthusiasm invested in its very successful first year (see pages 16-17); and finally to the members of our Advisory Board (see pages 18-19) for their very significant investment of time and effort as well as their very thoughtful and valuable consideration.

Sincerely,



Robert Harrison,
IACS Director



Lynn Allopenna,
IACS Administrative Director



Alan Calder,
IACS Deputy Director



PhD students and their advisors from all over the world attended the IACS MultiResolution Analysis summer camp held August 1-12, supported by NSF TESSE grant #1450344

VISION

Our vision is to be an internationally recognized center in data and computational science, having vibrant multidisciplinary research and education programs, with broad leadership and benefit across Stony Brook and SUNY, and with demonstrated economic benefit to New York State.

MISSION

To realize our vision we will:

- Advance the intellectual foundations of computation and data, with high-impact applications in engineering and the physical, environmental, life sciences and the humanities;
- Grow our faculty and students emphasizing excellence and diversity in coordination with academic units across Stony Brook and with Brookhaven National Laboratory;
- Build a highly-productive, multi-disciplinary and multi-cultural environment for research and education; and
- Grow our research programs and facilities, and establish regional, national and international partnerships with industry, government laboratories and academia.

We presently have 11 faculty spanning chemistry, materials by design, condensed matter, astrophysics, atmospheric science, nano-science, sociology, applied mathematics, and computer science. Another approximate 30 faculty are affiliated with the institute from diverse departments, and we are actively recruiting two senior endowed positions and two junior positions in computer science and applied mathematics.

We began with a transformational \$10 million anonymous donation plus matching funds of equal value from the Simons Foundation that enabled Stony Brook University to establish our institute. Our integrated, multidisciplinary team of faculty, students, and staff overcome the limitations at the very core of how we compute, collectively take on challenges of otherwise overwhelming complexity and scale, and individually and jointly define new frontiers and opportunities for discovery through computation.

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NEW HIRES



TONY CURTIS

Tony Curtis joined IACS in April 2016 as a Programming Project Leader, working with Professor Barbara Chapman's group. He has over 20 years professional experience in designing, implementing, managing and programming systems, primarily but not only in High Performance Computing, from departmental to national level scales. In that time he has developed extensive skills to understand how best to implement systems according to user community needs and how to develop the necessary infrastructure to maintain and future-proof an effective service environment. Recent work in the research world developing Partitioned Global Address Space libraries allows him to see computational needs from different perspectives and to integrate these different aspects of High Performance Computing.

ROSALIA DAVI

Rosalia Davi joined IACS in March 2016 as the Diversity Outreach Coordinator. Her primary focus is to grow the successful recruitment of underrepresented scholars for graduate and postdoctoral study across the STEM disciplines and more specifically for the institute's science domains. She has over five years of experience in higher education, specifically in experiential education, where she advised a highly diverse student and alumni population on professional, personal and civic development. Prior to her time in Student Affairs, Rosalia worked for a college access non-profit, helping to bridge the opportunity gap for under-resourced students through program management and fundraising. She has a dual master's degree in Gender and Cultural Studies and Communications Management from Simmons College, and is a Stony Brook University alumna.

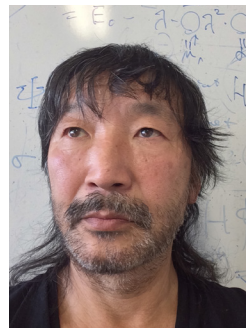


JEFFREY HEINZ

Professor Jeffrey Heinz will be coming to IACS as a core faculty member in the fall of 2017 from the Department of Linguistics and Cognitive Science at the University of Delaware. Heinz's research lies at the intersection of theoretical and mathematical linguistics, theoretical computer science, and computational learning theory, with specializations in phonology, linguistic typology, and grammatical inference. His work in these areas has appeared in the journals *Science*, *Linguistic Inquiry*, *Theoretical Computer Science*, *Topics in Cognitive Science*, and *Transactions of the Association of Computational Linguistics*, among others. The Linguistic Society of America recognized Heinz with its 2017 Early Career Award for his "contributions leading to a new computational science of inference and learning as applied to language."

ERIC ROSENBERG

Eric Rosenberg started with IACS in July of 2016 as a Senior HPC Engineer to help manage our on-campus computing clusters. He earned his Bachelor's of Technology with a concentration in Networking and Telecommunications from Briarcliffe College. After working in Cold Spring Harbor Laboratory for 2 years, he came to Stony Brook University in 2007. Since then, he's worked in the Client Support department, where he ran the walk-in center for students with software problems; and the Systems Support department, where he managed the campus Active Directory, VMware environment, storage area networks, file and printer sharing and various other systems language."



HIDEO SEKINO

Professor Hideo Sekino comes to IACS from the Toyohashi University of Technology in Japan. He originally was an IACS affiliate faculty member but became a part-time Research Professor with us in July 2016 to help foster the creation of international graduate exchange programs here at SBU. Professor Sekino's research is in molecular electronic structure with an emphasis on high-accuracy response properties. He contributes to the design and implementation of MADNESS and is also interested in relativistic and time-dependent methods.

NEW AFFILIATES



LILIANA DÁVALOS-ÁLVAREZ
Associate Professor
Ecology and Evolution
Stony Brook University



JANET NYE
Assistant Professor
School of Marine and Atmospheric Sciences
Stony Brook University



IL MEMMING PARK
Assistant Professor
Neurobiology and Behavior
Stony Brook University



CHRISTINE O'CONNELL
Assistant Professor and Associate Director
School of Journalism and Alan Alda Center for Communicating Science
Stony Brook University



IACS students and faculty mingle in a local pub at a get-together organized by the IACS Student Association. Photo by Taylor Ha

SEMINARS & EVENTS

IACS Seminar Series

February 4, 2016

Joel Saltz, Stony Brook University
Integrative Multi-scale Analysis in Biomedical Data Science: Tools, Methods and Challenges

February 18, 2016

William Tang, Princeton University
Scientific Software for Extreme Scale Applications in Fusion Energy R&D

February 25, 2016

Dima Kozakov, Stony Brook University
Modeling and Modulating Protein-Protein Interactions using High Performance Computing

March 3, 2016

Fotis Sotiropoulos, Stony Brook University
Immersed Boundary Methods for Simulating Fluid-Structure Interaction

March 8, 2016

Michele Benzi, Emory University
Walk-Based Measures of Centrality, Communicability, and Robustness in Networks

March 10, 2016

Scott Ferson, Applied Biomathematics
Non-Laplacian Uncertainty and Why Your Simulations Need to Tend to It Today

March 30, 2016

Cheng Wang, Xiaonan Tian, Rengan Xu, University of Houston
Implementing and Optimizing OpenACC on GPUs

March 31, 2016

Dongbin Xiu, Purdue University
Uncertainty Quantification Algorithms for Large-scale Systems

March 31, 2016

Il Memming Park, Stony Brook University
Inferring Local Cortical State from Neural Time Series



Dima Kozakov

April 7, 2016

Stephan Irle, Nagoya University
Ultrafast Linear Scaling Quantum Chemical Methods: Methodology and Applications to Problems in Materials Sciences

April 7, 2016

Huan Liu, Arizona State University
The Good, the Bad and the Ugly: Uncovering Novel Opportunities of Data Science

April 8, 2016

Hongyuan Zha, Georgia Institute of Technology
Modeling Asynchronous Event Dynamics

April 18, 2016

Richard Tapia, Rice University
Building a Culture of Diversity in Higher Education: Obstacles and Successes

April 27, 2016

Broxton Miles, University of Alabama
Dependence of Light-curves and Spectra on Metallicity in Type Ia Supernova Models

April 27, 2016

Roberto Car, Princeton University
Disordered Water Phases from Ambient to Ultrahigh Pressure

April 28, 2016

Thomas Graf, Stony Brook University
Computational Lessons From and For Language

May 17, 2016

Martin Deneroff, Emu Technology
The Emu Technology: Efficiency Through Thread Migration and Memory-Side Processing

September 15, 2016

Ann Almgren, Lawrence Berkeley National Laboratory
Next-Generation AMR

September 22, 2016

Krishna Kavi, University of North Texas
Computer Systems Research at the University of North Texas

October 19, 2016

Siddhartha Jana, University of Houston
Optimizations for Energy Efficiency for Distributed Memory Programming Models

November 3, 2016

Angela Shiflet, Wofford College
Computational Thinking: Applying Computer Science and Mathematics to Scientific Problems

November 7, 2016

Huan Liu, Arizona State University
Evaluation Dilemmas in Social Media Research



IACS Research Day 2016

November 11, 2016

Matthias Muller and Christian Terboven, Aachen University
HPC and Simulation Science at RWTH – Infrastructure, Applications and Programming Models

November 18, 2016

Yoshiki Kato, Toyohashi University of Technology
Molecular Activity Prediction using Deep Learning Software Library

November 29, 2016

Hongyuan Zha, Georgia Institute of Technology
Optimization and Intervention in Point Processes Networks with Application to Activity Shaping and Social Campaigning

December 1, 2016

Mark Ratner, Northwestern University
By Indirections Find Directions Out: Electronic Motion Within and Among Molecules

December 8, 2016

Valerio Pascucci, University of Utah
Multi-Scale Morse Theory for Science Discovery

Projects, Programs & Events

January 21, 2016

Introduction to MPI: a Hands-on Tutorial
Stony Brook University

April 5, 2016

XSEDE HPC Workshop: Big Data
Stony Brook University

April 8-11, 2016

Formalism and Hands-on Application of Ultrafast Linear-scaling, Massively Parallel Quantum Chemical Methods Based on Density-functional Tight-binding (DFTB) for Computational Materials Sciences
Stony Brook University/IACS

April 13, 2016

IACS Research Day
Stony Brook University/IACS

April 18, 2016

Drawing Diversity to Academia
Stony Brook University/IACS

May 24, 2016

OpenACC and GPU Hands-on Workshop
Stony Brook University/IACS

June 14-17, 2016

XSEDE Summer Boot Camp
Stony Brook University/IACS

July 11-20, 2016

IACS Computes! High School Summer Camp
Stony Brook University/IACS

August 1-12, 2016

MultiResolution Analysis (MRA) Summer School
Stony Brook University/IACS

August 18-19, 2016

Data Carpentry Workshop
Stony Brook University/IACS

August 22-26, 2016

Developing Models for Structure and Style in Scientific Writing
Stony Brook University/IACS

September 7-8, 2016

XSEDE HPC Workshop: MPI
Stony Brook University/IACS

September 10 & 17, 2016

Master Teacher workshop
Stony Brook University/IACS

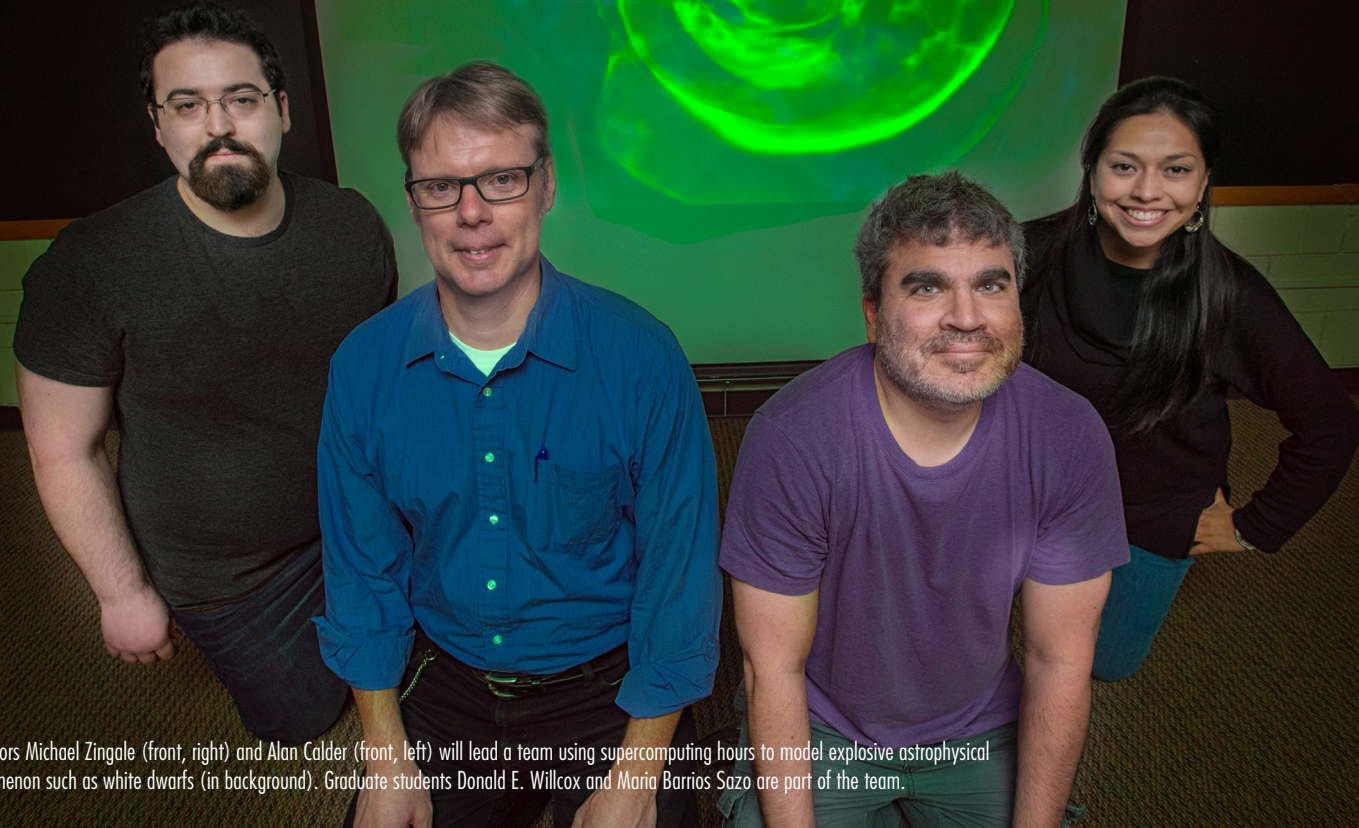
October 27, 2016

Andrew Sorensen Seminar and Performance
Stony Brook University/IACS

November 29, 2016

Conversation with Renaissance Technologies
Stony Brook University/IACS

INCITE



Professors Michael Zingale (front, right) and Alan Calder (front, left) will lead a team using supercomputing hours to model explosive astrophysical phenomenon such as white dwarfs (in background). Graduate students Donald E. Willcox and Maria Barrios Sazo are part of the team.

INCITE AWARD TO ADVANCE MODELING ASTROPHYSICAL EXPLOSIONS VIA SUPERCOMPUTING

A national research team led by Stony Brook University has been awarded 45 million hours on one of the world's fastest supercomputers, the Titan Cray XK7 at Oak Ridge National Laboratory, to further their research on explosive astrophysical phenomenon and model these complex occurrences by way of supercomputer-generated simulations. The award, sponsored by the U.S. Department of Energy's Office of Science through its Innovative and Novel Computational Impact on Theory and Experiment (INCITE) Program, recognizes national research projects with high potential for accelerating discovery.

The project, titled "Approaching Exascale Models of Astrophysical Explosions," is led by Michael Zingale, PhD, and Alan Calder, PhD, Stony Brook University Professors in the Department of Physics and Astronomy. The project is one of only six nationally in the area of astrophysics to be awarded by the 2017 INCITE Program. The team received a similar award for supercomputing hours in 2014.

The research team will carry out a comprehensive study of stellar explosions and their precursors using a suite of simulation codes. The collaboration will study a host of astrophysics problems, and of particular interest to the Stony Brook team are problems powered by fusion reactions.

"The award and our continued use and development of simulations using this world-renowned supercomputer will further advance our understanding of astrophysical explosions," said Professor Calder, also an affiliate of the Institute for Advanced Computational Science (IACS) at Stony Brook.

Professor Calder added that more specifically, the team will investigate problems involving explosions occurring either on the surface or the interior of compact stars. For example, if a compact star, a white dwarf or a neutron star, gains material on its surface from a companion star, then that surface layer can suddenly experience a thermonuclear runaway and explode. Or, in the case of a white dwarf, the whole star can explode.

"The supercomputer hours broadens our ability to explore a multitude of configurations of these stellar explosions," explained Professor Zingale, also an affiliate of IACS. "Our focus will be on X-ray bursts, which are a layer of transferred material on the surface of a neutron star that explodes, and thermonuclear supernovae, the explosion of a white dwarf star."

Both Professors Calder and Zingale have received supercomputer hours from numerous INCITE program awards in previous years. Two graduate students from the Department of Physics and Astronomy, Maria Barrios Sazo and Donald E. Willcox, will be part of the research team for the 2017 award.

The project also includes co-investigators from Lawrence Berkeley National Laboratory, Oak Ridge National Laboratory, the University of California, Los Alamos National Laboratory, and the University of Tennessee.

The INCITE Program promotes transformational advances in science and technology through large allocations of time on state-of-the-art supercomputers.

STRIDE



L-R Back row: IACS and STRIDE PI Robert Harrison, CoPIs Arie Kaufman, Janet Nye. Front row: CoPIs Liliana Davalos, Heather Lynch, Christine O'Connell. CoPIs not pictured: Erez Zadok, Minghua Zhang, Joel Saltz

\$3M NSF GRANT WILL FUND PHD STUDENT TRAINING IN DATA ANALYTICS, VISUALIZATION AND SCIENCE COMMUNICATION



The Institute for Advanced Computational Science (IACS) has been awarded a five-year \$3M National Science Foundation Research Traineeship (NRT) grant to support graduate students from the departments of Applied Mathematics and Statistics, Biomedical Informatics, Computer Science, Ecology and Evolution, and the schools of Journalism and Marine and Atmospheric Sciences. This unique and interdisciplinary grant is for Science Training & Research to Inform DECisions (STRIDE). The award will prepare the next generation of scientists working with big data to support complex decision-making.

STRIDE is an innovative training program that will provide STEM graduate students with unique interdisciplinary skills to assist, create, and eventually lead the translation of complex data-enabled research into informed decisions and sound policies. These include skills traditionally taught to science students such as data analytics and visualization. The unique contribution of STRIDE is to also prepare scientists by building skills in decision support that are often not explicitly taught, such as understanding the perspectives of various stakeholders, science communication, and translating scientific uncertainty.

IACS Director Robert Harrison is the PI for this project: "Decision support and all of the skills it entails are essential for high impact science, and this need cuts across many disciplines. Our team is really excited about how this project will transform both our university and especially the careers and leadership opportunities for our students."

The training program encompasses spatial data, advanced visual data analytics, and high-performance and data-centric computing. Uniquely, the program also incorporates a domain discipline, science communication, including interpersonal skills and modern media (at the Alda Center for Communicating Science), as well as and decision-making. It also offers relevant internships at Department of Energy laboratories, IBM and NOAA.

The interdisciplinary nature of STRIDE is reflected in the faculty involved. The Co-PIs are: Liliana Davalos, associate professor, Ecology and Evolution; Arie Kaufman, distinguished professor and chair, Computer Science; Heather Lynch, associate professor, Ecology and Evolution; Janet Nye, assistant professor, School of Marine and Atmospheric Sciences; Christine O'Connell, associate director, Alan Alda Center for Communicating Science and assistant professor, School of Journalism; Joel Saltz, Cherith professor and founding chair, Biomedical Informatics; Erez Zadok, professor, Computer Science; and Minghua Zhang, professor, School of Marine and Atmospheric Sciences.

"We are thrilled to be part of this exciting collaboration and work with fellows to help them communicate complex data science to decision makers, especially on health and environmental issues where it is crucial that policy and management decisions be based on sound science," said Alda Center Associate Director Christine O'Connell.



REZAUL CHOWDHURY RECEIVES NSF CAREER AWARD FOR PARALLEL ALGORITHMS RESEARCH

Used with permission from the Department of Computer Science

Rezaul Chowdhury, PhD, an Assistant Professor in the Department of Computer Science in the College of Engineering and Applied Sciences, has received the prestigious Faculty Early Career Development (CAREER) Award from the National Science Foundation (NSF). The award will help to advance his research on developing theories and efficient tools to facilitate the design of portable parallel algorithms to be used in computing platforms ranging from small laptop computers to massive supercomputers. These algorithms will have no need of hardware parameters in the code, yet run efficiently.

The NSF CAREER Award is given to promising young university faculty nationwide who exemplify the role of teacher-scholar through outstanding research, excellent education and the integration of both education and research.

Dr. Chowdhury, who holds a joint appointment with Stony Brook's Institute for Advanced Computational Science (IACS), and advises Stony Brook's competitive programming teams for algorithmic problem solving, will receive \$535,000 over the next five years for the project, titled "A Unified Framework for Designing Efficient Resource-Oblivious Parallel Algorithms."

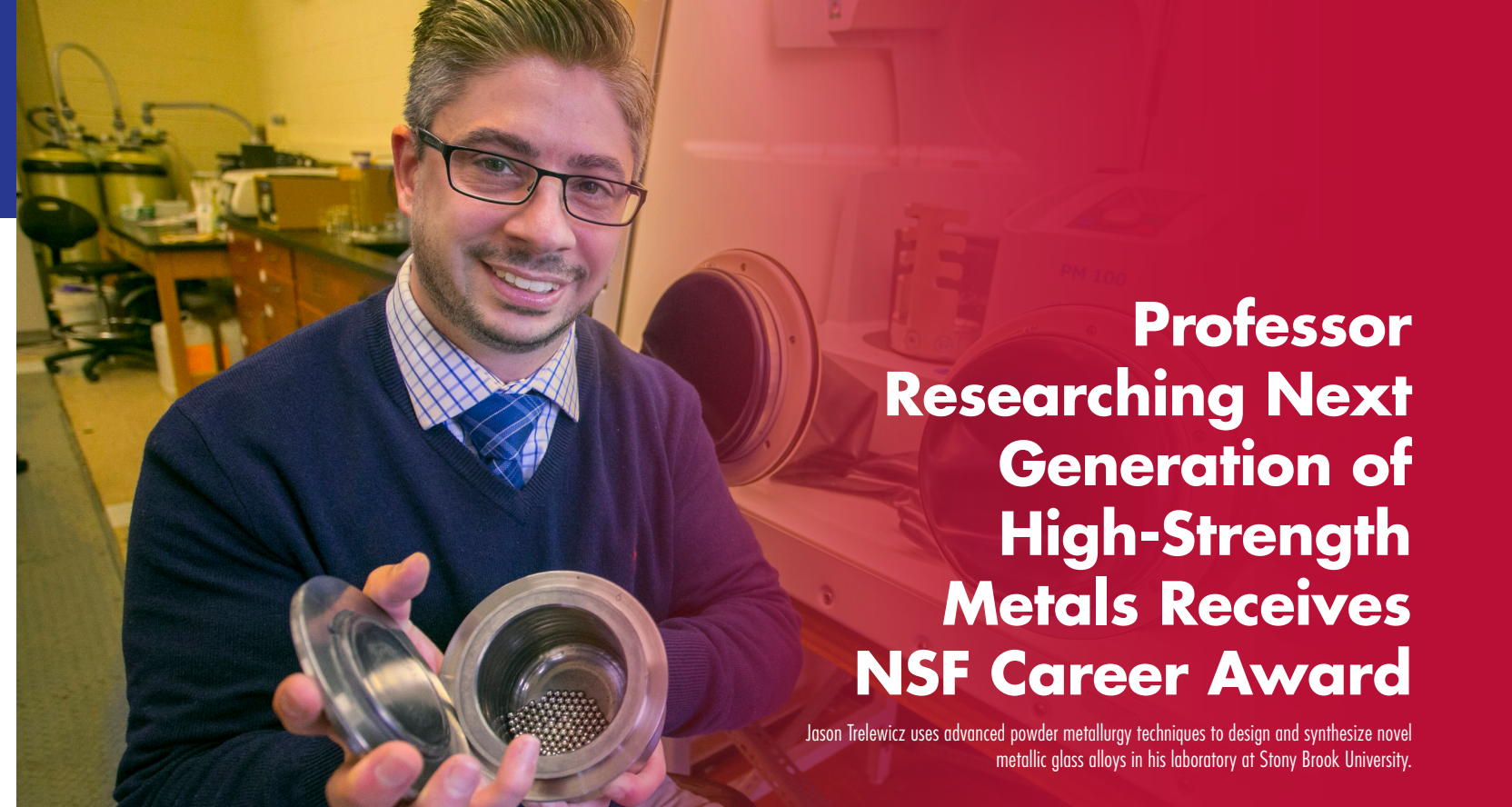
"The goal of the project is to shield programmers from the complicated details of the ever-changing underlying hardware platforms while still allowing them to write efficient parallel code," explained Dr. Chowdhury. "As a result of the research, we hope parallel programming will become simpler for most computers and supercomputers and no longer remain the domain of a few experts."

He also expects that a variety of computational science applications – ranging across physics, biology, chemistry, energy, climate, mechanical and electrical engineering and other areas – will become easier to develop and maintain with resource-oblivious parallel algorithms.

The results of the work will be disseminated through a new graduate course on portable algorithms, existing courses on analysis of algorithms, parallel programming and supercomputing, as well as workshops for students and professionals arranged through IACS.

Dr. Chowdhury received his PhD in Computer Science from the University of Texas at Austin. Before joining Stony Brook University in 2011, he worked as a postdoctoral researcher at UT Austin's Institute for Computational Engineering and Sciences (ICES), Boston University's Department of Biomedical Engineering (BME), and MIT's Computer Science and Artificial Intelligence Laboratory (CSAIL).

"As a result of the research, we hope parallel programming will become simpler for most computers and supercomputers and no longer remain the domain of a few experts."



Professor Researching Next Generation of High-Strength Metals Receives NSF Career Award

Jason Trelewicz uses advanced powder metallurgy techniques to design and synthesize novel metallic glass alloys in his laboratory at Stony Brook University.

The grant supports Jason Trelewicz's work that may impact the electronics, automotive and aerospace industries

by Greg Filiano – Jason Trelewicz, PhD, an Assistant Professor of Materials Science and Engineering at Stony Brook University (SBU), has received the prestigious Faculty Early Career Development (CAREER) Award from the National Science Foundation (NSF). The award will help to advance his research aimed at transforming applications of high-strength metals.

Trelewicz, a member of the College of Engineering and Applied Sciences (CEAS), will receive NSF CAREER funding of \$500,000 over the next five years to support his project, titled "Interface Engineered Amorphous Alloys for Thermoplastic Forming of Ductile Bulk Metallic Glasses."

According to the NSF, the CAREER Award is given to promising young university faculty who exemplify the role of teacher-scholar through outstanding research, excellent education and the integration of both education and research.

Trelewicz' research centers on the design, synthesis, and characterization of nanostructured and amorphous metals through computational modeling and materials science experimentation. Commonplace metals such as aluminum or steel are made up of atoms that are arranged in a regular, periodic structure. Amorphous metals on the other hand, exhibit a highly disordered atomic structure akin to a glass, and are consequently referred to as metallic glasses.

This relatively new class of materials, often used in products such as USB drives, medical and sporting equipment, has shown great promise as next-generation high-strength materials with applications in the electronics, automotive and aerospace industries. A problem that continues to plague metallic glasses is that they tend to be very brittle and can fail catastrophically. Processing routes for bulk manufacturing of these materials are also quite limited.

Trelewicz hopes to turn these problems with metallic glasses into opportunities for improvement with his new research. Under the NSF CAREER program, he will use atomistic simulations to design, atom-by-atom, novel interface engineered amorphous alloys. These

alloys will be manufactured and characterized to develop a new understanding of the deformation mechanisms at the nanoscale.

"The goal of the research will be to engineer interfaces into metallic glasses to enhance their strength, toughness, and formability," said Trelewicz. "Using integrated materials engineering principles, we will design novel metallic glasses with superior properties that can be manufactured at large-scales."

"Being recognized with the prestigious CAREER Award speaks volumes about Jason's research vision," said CEAS Dean Fotis Sotiropoulos. "This funding enables him to integrate research topics on the unique properties of metallic glasses into the undergraduate Material Science curricula offered by CEAS. It also provides an opportunity to engage underrepresented students and regional high schools in cutting-edge research."

The broader impact of the research, says Trelewicz, is that society will be greatly impacted by metallic glasses that can be manufactured and optimized for applications as advanced structural and electronic materials.

"These materials have the potential to revolutionize sheet metal production used in industries that transform the ways we travel, build, and communicate," he explained.

A faculty member at Stony Brook since 2012, Trelewicz is the Director of the Engineered Metallic Nanostructures Laboratory, an affiliated faculty member with the Institute for Advanced Computational Science, and he is the Director of the NYSTAR-funded High Performance Computing Consortium at SBU.

Trelewicz earned his PhD in Materials Science and Engineering from Massachusetts Institute of Technology in 2008. Prior to joining the faculty at Stony Brook, he was a Research Director at MesoScribe Technologies, Inc. He is the recipient of the 2015 Young Leader Professional Development Award and 2014 Emerging Leaders Alliance Award from The Minerals, Metals, and Materials Society (TMS), and received the Top Speaker Award at the 2010 Defense Manufacturing Conference.

DIVERSITY



DRAWING DIVERSITY TO ACADEMIA

Increasing diversity at IACS has been at the forefront of our efforts this past year. In April we organized and hosted Drawing Diversity to Academia, a panel discussion that featured an array of experts from Stony Brook University and beyond. The session was designed to discuss opportunities, best practices and novel ideas for increasing the participation and success of underrepresented minorities in the STEM fields.

Participants included IACS Director Robert Harrison, who chaired the event, as well as Dennis Assanis, former Provost, SBU; Noel Blackburn, Manager, University Relations and DOE Programs, Brookhaven National Laboratory; Frances Brisbane, Vice President for Health Sciences Workforce Diversity, SBU; Carlos Medina, Chief Diversity Officer and Senior Associate Vice Chancellor for Diversity, Equity and Inclusion, SUNY; Charles Robbins, Vice Provost for Undergraduate Education and Dean of the Undergraduate Colleges, SBU; Toni Sperzel, Assistant Dean, Center for Inclusive Education; Charles Taber, Dean of the Graduate School and Vice Provost for Graduate Education, SBU; and Richard Tapia, Professor & Director, Center for Excellence and Equity in Education, Rice University.

"It was truly a pleasure to have participated on such an important panel and topic of discussion," Carlos Medina said. "Given our current demographics, higher education leaders need to work across their respective institutions to create a welcoming and inclusive culture for all."

The panel discussion was followed by Richard Tapia speaking on Building a Culture of Diversity in Higher Education as part of the Provost's Lecture Series. He focused on obstacles that universities must overcome to improve representation at the graduate and faculty levels, and he shared his own personal journey - from being born to Mexican immigrants in Los Angeles to making a trip to the White House to receive the National Medal of Science.



ENGAGING WITH PURCHASE

In July, IACS Director Robert Harrison (back row, fourth from left) visited Purchase University, specifically to talk with students engaged in the Bridges to the Baccalaureate Summer Program Community College Day, which aims to provide support to underrepresented minority students studying science.

Picture provided by Professor Joseph Skrivanek



WOMEN IN COMPUTING

IACS Diversity Outreach Coordinator Rosalia Davi along with IACS Associate Professor Marivi Fernández-Serra attended the Grace Hopper Celebration of Women in Computing in Houston, TX, which was attended by over 11,000 people from more than 63 countries.

Women came from all around the globe to learn, exchange ideas, and be inspired. Rosalia and Marivi spoke with a whole host of graduate and undergraduate students interested in academic and research opportunities at Stony Brook University. "It was fantastic to meet

these students, and we also met many women who were alumni of SBU who are now working in high-tech companies like Facebook, Google, Amazon, Intel, IBM, etc.," said Professor Serra. On the very last day of the conference all these bright and inspirational SBU alumni gathered together at the booth to take a picture. It was certainly a successful celebration of women in computing and technology, and Stony Brook did not pass unnoticed!

TAPIA CELEBRATION

This past fall IACS made its first foray into recruiting at a national conference by sending IACS Diversity Outreach Coordinator Rosalia Davi and IACS Student Diversity Ambassador Adrián Soto to the ACM Richard Tapia Celebration of Diversity in Computing conference in Austin, TX. Their goals were to meet and greet undergraduate students from around the country in hopes of finding those who could join the elite group of graduate students here at IACS.

Of the 950 attendees, about 850 were students, and those of whom stopped by the IACS booth hailed from universities across the country: University of Georgia, Bard, Harvard, U of Michigan - Ann Arbor, Purdue, Williams, Temple, UC Berkeley, Arizona State, MIT, and Cornell to name a few. According to Davi, "Each student we met with has enormous potential to be successful in his/her field, while also impacting society (and STEM) positively."



IACS Diversity Outreach Coordinator Rosalia Davi (second from the left) and IACS Student Diversity Ambassador Adrián Soto (far left) at the ACM Richard Tapia Celebration of Diversity in Computing conference in Austin, TX. IACS Professor Barbara Chapman (second from the right) attended as well as a representative for Brookhaven National Laboratory, where she holds a joint appointment. Picture courtesy of ACM Richard Tapia Celebration of Diversity in Computing Conference



A MESSAGE FROM HPC^{NY} DIRECTOR AT SBU PROFESSOR JASON TRELEWICZ

HPC^{NY} has achieved over \$33M in documented economic impacts leading to the creation and retention of just over 100 jobs working with 28 partner companies.

Since its formation in 2008, New York's High Performance Computing consortium (HPC^{NY}) has grown from an innovative and ambitious idea into a unique and well-established resource for solving some of the most complex design, modeling, and performance challenges facing New York State companies. HPC^{NY} is the only entity of its kind in the public and private sector working to match cutting-edge high-performance computing research to modern day industrial challenges. One of the characteristics that distinguishes the HPC^{NY} consortium from other university consortia is our interactions and collaborations with industry. We are excited by the real-world challenges that are presented to us, and we take great pride in our ability to solve the problems and meet the needs of our industrial partners.

Over the past year, the team at Stony Brook University has forged ahead on enhancing the technical state of our HPC^{NY} projects by leveraging the scientific computing expertise of our faculty with the Lfred cluster, made possible through funding from New York State's Long Island Research and Economic Development Council. In collaboration with our industrial partners, focus has been placed on accelerating the design, testing, and optimization of materials and products by applying advanced modeling and simulation techniques. From these activities, significant economic impacts have been produced over the past year alone and include \$3.9M in federal and private funding, \$500K in cost savings, and 10 jobs being created and/or retained across the various Long Island facilities. When combined with contributions from other consortium members and taken collectively over the entire duration of the consortium, HPC^{NY} has achieved over \$33M in documented economic impacts leading to the creation and retention of just over 100 jobs working with 28 partner companies.

Success of the HPC^{NY} consortium is directly connected to the accomplishments of our industrial partners, as documented through our HPC^{NY} success stories. One such new success story is Professor Dilip Gersappe's collaboration with EOS Energy Systems. EOS'

mission is to develop cost-effective energy storage solutions that are not only less expensive than other battery technologies but also less expensive than most economical alternatives used today to provide the same services. Lattice Boltzmann modeling was employed by Prof. Gersappe's group to understand the key mechanisms that control the operation of hybrid battery technologies. Particular focus was on mitigating the formation of dendrites, illustrated in Figure 1, that limit the capacity and life of zinc-hybrid batteries through charge-discharge cycles. From this collaboration, new operating maps were established to predict dendrite formation as a function of charging rate and other system parameters. Dr. George Adamson, VP for Research and Development at EOS Energy, stated, "Our collaboration with HPC^{NY} has provided EOS Energy Storage with valuable scientific information regarding the design and engineering of our battery. The computer modeling results have allowed EOS to find optimal operating conditions for our commercial battery, which will in turn make our batteries more efficient for grid storage applications in the future."

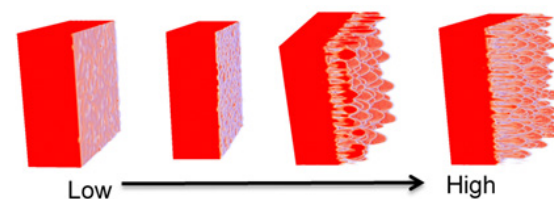


Figure 1: Dendrite formation in a zinc-hybrid cathode system as a function of increasing charging rate

As we look to the future of the HPC^{NY}, we are working with our consortium partners to secure funding from New York State for continued success of the HPC^{NY} model. An ambitious plan has been outlined to double the number of industry collaborations and expand into new fields of expertise, which will propel economic growth in New York State by tripling our economic impacts. We have an exciting year ahead as we develop new industrial engagements, and any faculty members working with industry interested in teaming with HPC^{NY} are encouraged to visit our website <https://hpc-ny.org/> and contact Jason.Trelewicz@stonybrook.edu.



SEAWULF AWAKENS

The new SeaWulf cluster came alive in April of 2016 in the Computing Center at Stony Brook University. This cluster was purchased as a result of a Major Research Instrumentation grant awarded to IACS from the National Science Foundation (NSF). The award consisted of \$1.4M from NSF with a \$300K match being applied internally from the following departments:

- Applied Mathematics and Statistics Department
- College of Engineering and Applied Sciences
- College of Arts and Sciences
- Division of Information Technology
- Ecology & Evolution Department
- Laufer Center for Physical and Quantitative Biology
- Materials Science and Chemical Engineering Department
- Mechanical Engineering Department
- Office of the Vice President for Research
- Physics and Astronomy Department
- Provost's Office
- School of Marine and Atmospheric Sciences

A special note of thanks also goes to Empire State Development's Division of Science, Technology and Innovation (NYSTAR) program, which awarded us another \$300K match, bringing the total investment to \$2M.

This highly-extensible system seeded an institutional approach to research computing that has provided and continues to provide great cost savings across SBU, and the cluster increases the overall quality and functionality of the research cyber infrastructure. The system delivers a roughly 50-fold increase in capability over the original SeaWulf system from 2006.

The cluster is used for research as well as deep training opportunities for undergraduate and graduate students. The system boasts 86 users as well as three currently active classes running the gamut from Applied Mathematics to Biology. The system is also being used extensively for New York's High Performance Computing Consortium (HPC^{NY}) program, a "unique and well-established resource for solving some of the most complex design, modeling, and performance challenges facing New York State companies." (See the article on page 14.)

SeaWulf Specs

- 164 compute nodes, each with two Intel Xeon E5-2683v3 CPUs
- 8 of the compute nodes contain 4 GPUs each
- Total of 32 x Nvidia Tesla K80 Accelerators, offering 64x GK210 (K40) Cores (159,744 CUDA cores)
- CPUs offer 14 cores each and operate at a base speed of 2.0 Gigahertz.
- Each node has 128 Gigabytes of DDR4 Memory
- The nodes are interconnected via a high-speed network operating at 40 Gigabits per second, allowing transfer of ~5 Gigabytes of data each second.
- The storage array is comprised of 180x 6 Terabyte nearline SAS disks IB-attached to two Network Shared Disk servers, and 5x 1,600 Gigabyte Solid State Disks acting as the metadata pool for the GPFS. This storage system can provide sustained

- 4k Random Read Input Output Operations per Second over 13,000*, and can sustain sequential transfers at over 14 Gigabytes per second
 - The Cloud Component of the cluster is provided by 3 OpenStack Controllers orchestrating up to 20% of the compute nodes as hyper-visors to host virtual machines instantiated via the Self-Service Portal
- *RAID6 (8+2) x 180 drives, in a 4k Random Read scenario comprised of 99% Reads, QD=1, 32 threads



IACS STUDENT ASSOCIATION

Institute for
Advanced
Computational
Science



“Being involved in IACS means you are constantly networking and collaborating with students from all different scientific backgrounds. The peer review system we put in place has helped students gear their research presentations to a broad audience with diverse interests.”
IACS Student Association Secretary Joel Anderson

(L-R) IACS Student Association Treasurer Tristan Delaney, President Aimilios Sofianopoulos, and Secretary Joel Anderson stand outside the entrance to IACS. Not pictured: Vice President Mohammad Mahdi Javanmard
Photo by Taylor Ha

In an effort to create a pipeline of social and professional development activities for anyone interested in computational science, a group of IACS PhD students came together in late 2015 to form the IACS Student Association. Their first full year was an unequivocal success: They organized a wide range of events from social get-togethers to informative brown bag lunches, and they received official SBU club status.

One of their premier sponsored events was inviting and hosting a world-renowned Provost Lecture Series speaker, Professor Jack Dongarra from the University of Tennessee and Oak Ridge National Laboratory. The Association not only brought together a crowd of over 100 people for Dongarra’s lecture, they also arranged for one-on-one meetings between faculty and staff; organized an afternoon of research presentations from students; and coordinated a dinner for faculty and students with Dongarra as the guest of honor. “Jack Dongarra is one of the most highly cited computer scientists in the world. He gave an inspiring talk and shared invaluable insights with the students who presented their research to him. It was a great accomplishment for our association to be able to host his visit,” said association VP Mahdi Javanmard.

With official club status comes potential funding from the Graduate Student Organization (GSO) and Faculty Student Association to subsidize the costs associated with organizing events. “Financial assistance from the GSO makes it possible for our club to host events which benefit IACS students and the Stony

Brook University community as a whole. We were really grateful when the GSO helped us with getting Professor Dongarra to speak at the Provost Lecture Series in November,” said Treasurer Tristan Delaney.

Another particularly noteworthy event was the Student/Faculty Dinner, the “crown jewel of our events” said President Aimilios Sofianopoulos. The dinner was held off campus at a local restaurant that afforded IACS faculty and students the chance to dine together in a relaxed environment, to exchange ideas, and get to know each other outside of work. “I want to try and create a small community here,” said Sofianopoulos. “I believe this dinner was a good start.”

The student association was also instrumental in initiating the IACS Student Seminar Series. Core and affiliate faculty are encouraged to nominate a student from their group to give a seminar on their research in a 30-minute presentation. Three days before the student is due to present, the speaker is invited to ‘test-run’ the presentation to a small group of students made up of association members along with a rotating group of students who are slated to speak later that same semester. “Being involved in IACS means you are constantly networking and collaborating with students from

all different scientific backgrounds. The peer review system we put in place has helped students gear their research presentations to a broad audience with diverse interests. The ‘practice sessions’ also give the presenters a level of confidence they might not have had without the constructive input from the peer group,” said association Secretary Joel Anderson.

More information about the IACS Student Association can be found on their website: <http://you.stonybrook.edu/iacssa/contact/> and on their Facebook page called “IACS Student Association.”



STUDENT ASSOCIATION

Events

January 21, 2016
Introduction to MPI: a Hands-on Tutorial
Stony Brook University

January 21, 2016
Movie Night
Stony Brook University

March 10, 2016
Spring Break Warmup

April 28, 2016
Student-Faculty Dinner
Pentimentos

September 22, 2016
IACS 2nd Annual Apps & Ale Social
Bench Bar & Grill

October 18, 2016
IACS Brown Bag Lunch
Cluster Etiquette

November 8, 2016
IACS Brown Bag Lunch
Bash Scripting for Fun and Profit

November 10, 2016
Jack Dongarra, University of Tennessee/ORNL
Provost’s Lecture Series

STUDENT ASSOCIATION

Seminar Series

February 3, 2016
Dan Elton, Physics & Astronomy
Propagating Optical-Phonon Like Modes in Liquid Water

February 10, 2016
Aimilios Sofianopoulos, Mechanical Engineering
Computational Fluid Dynamics Simulation of Natural Gas Combustion in a Spark Ignition (SI) Engine

February 24, 2016
Bin Cheng, Materials Science & Engineering
Plastic Strain Accommodation in Crystalline-Amorphous Nanolaminates containing Columnar Nanograins Quantified through Continuum Deformation Metrics

March 23, 2016
Rebecca Conley, Applied Math & Statistics
Overcoming Element-Shape Dependence of Finite Elements with Adaptive Extended Stencil FEM

April 6, 2016
Pramod Ganapathi, Computer Science
Autogen: Automatic Discovery of Cache-Oblivious Parallel Recursive Algorithms for Solving Dynamic Programs

September 28, 2016
Verinder S. Rana, Applied Math & Statistics
Uncertainty Quantification and Sensitivity Analysis for Inertial Confinement Fusion Simulations

October 5, 2016
Vivek Kulkarni, Computer Science
Modeling Linguistic Variation in Online Social Media

October 10, 2016
Bento Goncalves, Ecology & Evolution
Autonomous Satellite-based Surveys of Antarctic Seals Using Multi-scale Convolutional Neural Networks

November 2, 2016
Zeyang Ye, Applied Math & Statistics
Parallelization of Markov Chain Monte Carlo Methods

November 16, 2016
Longtao Han, Materials Science & Engineering
Migration of Carbon Adatom on a Charged Single Walled Carbon Nanotube

November 28, 2016
Mozhgan Rahimi Boldaji, Mechanical Engineering
Computational Fluid Dynamics Simulation of the Effects of Direct Water Injection on Advanced Combustion

December 7, 2016
Alexander Nodeland, Applied Math & Statistics
Optimal Wavelet Bases for Audio Compression

IT'S OFFICIAL: IACS STUDENT ASSOCIATION HAS A BANNER FIRST YEAR

ADVISORY BOARD RECOGNIZES "STRONG SPIRIT" IN IACS

The Board

The second meeting of the IACS Advisory Board was held on September 9, 2016.

The participating Board members were:

- Professor Mary Hall, University of Utah
- Professor David Keyes, KAUST and Columbia University
- Dr. Lois McInnes, Argonne National Laboratory
- Dr. Wolfgang Wander, Renaissance Technologies LLC
- Professor Margaret Wright, New York University
- Professor Michael Macy, Cornell University

The Meeting

Preceding the meeting was dinner the evening before with Engineering & Applied Sciences Dean Fotis Sotiropoulos, Arts & Sciences Dean Sacha Kopp, and Marine and Atmospheric Sciences Interim Dean Larry Swanson welcoming the panel at a lovely dinner at the Fifth Season in Port Jefferson.

On the day of, the review began with a welcome from Vice Provost for Faculty Affairs Stella Tsirka. IACS Director Robert Harrison then started the presentations with a reading of the charge to the Board:

- To review the institute's activities and accomplishments
- To make observations and recommendations for the success and impact of IACS
- To comment on the format and content of the Advisory Board meeting
- To provide feedback to the institute's members and university leadership

The day featured events intended to facilitate this charge, including presentations by Director Harrison, core faculty members, and students. Presenting faculty were Barbara Chapman, Matt Reuter, and Marat Khairoutdinov, and presenting graduate students were Aimilios Sofianopoulos and Aditi Ghai. Also student posters were displayed for viewing during lunch followed by members of the panel meeting individually with faculty. The panel had a closed-door session for discussion and then over the course of the next few weeks, the board put together a detailed report that was then provided to IACS leadership.

The Report

The report highlighted IACS accomplishments, including faculty awards and faculty and student publications, and noted the steady increase in number and size of grant submissions. The board praised the educational programs offered by IACS and extolled the "good fortune" and "strong spirit" of IACS students. They also noted the "rich and diverse" set of industry collaborations, IACS involvement with New York State initiatives, and commended IACS outreach efforts. Finally, the summary commented that IACS has "created a community among different disciplinary constituents of the University" and is thereby "augmenting the curriculum of the University in ways that respond to growing opportunities for large-scale simulation and large-scale data analytics," exactly the hope of IACS.

Recommendations

The board recommended suggestions for implementing the strategic plan and noted that IACS is best suited for data analytics, a computational process composed of algorithmic approaches to data, and suggested refining the strategic plan accordingly to sharpen the IACS role. The report also noted that an issue to be resolved concerns the social science component of IACS and that future plans to hire in this field would thereby allow computational social science to thrive.

The report also encouraged continued effort in senior hires and the education program, specifically maintaining the push to have the Graduate Certificate in Data and Computation for Scientists and Engineers officially approved and implemented. Finally, the report offered specific suggestions to continue the "branding" of IACS, including maintaining open-source software, leading specialist programs, and competing for major prizes.

IACS Advisory Board



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Sociology Department
Cornell University



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Biology Department
Harvard University



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Research Center
King Abdullah University of
Science and Technology



**PROFESSOR
MARGARET WRIGHT**
Computer Science Department
New York University

AWARDS

JR. RESEARCHER AWARD

Philip McDowell, Ecology & Evolution – Lynch
Adrián Soto, Physics & Astronomy – Fernández-Serra
Aditi Ghai, Applied Math & Statistics – Jiao
Zeyang Ye, Applied Math & Statistics – Deng

TRAVEL AWARD

Tristan Delaney, Applied Math & Statistics – Jiao
Javier Dominguez-Gutierrez, IACS – Krstic
Pramod Ganapathi, Computer Science – Chowdhury
Maureen Lynch, Ecology & Evolution – Lynch
Jun Ma, Applied Math & Statistics – Samulyak
Aimilios Sofianopoulos, Mechanical Engineering – Mamalis
Casey Youngflesh, Ecology & Evolution – Lynch

NEW RECRUIT AWARD

Eric Raut, Applied Math & Statistics

YOUNG WRITER'S AWARD

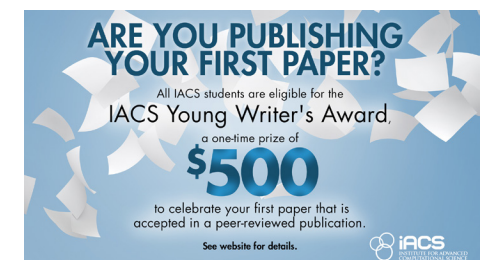
Bin Cheng, Materials Science & Engineering – Trelewicz
Simon Divilov, Physics & Astronomy – Fernández-Serra
Dzmitry Padhorny, Applied Math & Statistics – Kozakov
Donald Willcox, Physics & Astronomy – Calder
Maximilian Katz, Physics & Astronomy – Zingale
Nicole Bender, Ecology & Evolution – Lynch
Junting Ye, Computer Science – Akoglu
Hongxu Liu, Applied Math & Statistics – Jiao
Lukasz Orłowski, Applied Math & Statistics – Michalewicz
Emaad Ahmed Manzoor, Computer Science – Akoglu
Adrián Soto, Physics & Astronomy – Fernández-Serra

FUNDING SOURCES



We gratefully thank our supporters, particularly our generous donors (\$10M from an anonymous source matched by \$10M from the Simons Foundation) for making 2016 a wonderful year for IACS. Through the support from both our donors and the University, we were able to achieve many of our projected goals from last year, and we continue to grow and progress, making it a bright future for computational science at SBU and beyond. As a result of this support, in 2016 we accomplished the following:

- Supported travel for 7 national and international visitors to the Institute
- Hosted 28 speakers in our seminar series on a range of topics from linguistics to the physical sciences to Antarctic wildlife - of special note were invited guests Roberto Car from Princeton and Mark Ratner from Northwestern University
- Held our first Faculty Retreat for both core and affiliate faculty with 40 in attendance and with select presentations from OVPR, HPC^{NY} and Research Computing
- Endorsed the IACS Student Association's first year of events:
 - Hosting 5 social and professional development gatherings
 - Working with the Provost's office to invite and schedule a day of faculty/student interactions and a Provost's Lecture Series seminar with Prof. Jack Dongarra from the University of Tennessee, Knoxville and Oak Ridge National Laboratory
 - Starting the IACS Student Seminar Series this year with 12 students presenting their work to an audience of their peers
 - Starting a voluntary peer review process for all student seminar speakers
- Successfully ran our second annual IACS Computes! high-school summer camp with an increase from 10 to 14 students
- Supported two new Python programming camps: One for Master HS Teachers from the local area; one for HS students specific to the Port Jefferson and Mount Sinai school districts
- Hired (jointly with the Center for Inclusive Education) a Diversity Outreach Coordinator
- Hired (jointly with the Linguistics Department) a new faculty member
- Hired (jointly with the Department of Information Technology) a new Systems Administrator
- Held 8 programming workshops and our annual writing course
- Awarded 4 Junior Researcher Awards; 1 New Recruit Award; 11 Young Writer Awards, and 7 Travel Awards
- Submitted and are awaiting approval from the NY State Education Department for our 17-credit Certificate in Data and Computation for Scientists and Engineers (CDCSE)
- Submitted and are awaiting approval from the SBU Graduate Council for our 15-credit, NSF-supported STRIDE advanced graduate certificate
- Continued our support of the Center for Inclusive Education with \$12.5K to help defray costs associated with increasing diversity in the STEM fields
- Brought online a second computational cluster, 164-node SeaWulf
- Collaborated, trained and supported 2 high school students, one Fulbright fellow, and two graduate interns



We continue to move forward with this year's primary goals of:

- Finish the recruiting and installing of our two endowed chair positions
- Successfully undergo our first 5-year review
- Officially register and advise CDCSE students
- Hire a STRIDE NSF grant administrator
- Work with Dr. Melissa Woo, the west campus CIO and DoIT staff to facilitate SBU-wide research computing on campus
- Continue to build a world-class computational infrastructure with technical support to free faculty and students to focus on creativity and innovation

Interested in investing in Stony Brook University?
 Call 631-632-6330 or visit stonybrook.edu/foundation

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FACULTY



1. ALAN CALDER

Alan Calder is an associate professor in the Department of Physics and Astronomy at SBU. His research is in the field of nuclear astrophysics, and his work involves simulating explosive astrophysical phenomena, principally bright stellar explosions known as supernovae. He is also interested in the underlying physics of these events and in methodology for Verification, Validation, and Uncertainty Quantification of simulations and models. He obtained his PhD from Vanderbilt University and prior to coming to Stony Brook, he held research appointments at the National Center for Supercomputing Applications and the University of Chicago.

2. BARBARA CHAPMAN

Barbara Chapman joined SBU in September 2015 as an IACS core faculty member and a professor in AMS. She is a native of New Zealand who studied Mathematics and Computer Science in her home country, Germany and Northern Ireland, where she completed her PhD on software support for distributed memory programming. She has been engaged in research on parallel programming languages and compiler technology for more than 15 years. Prior to coming to Stony Brook, her research group at the University of Houston developed OpenUH, a state-of-the-art open source compiler that is used to explore language, compiler and runtime techniques, with a special focus on multi-threaded programming. Dr. Chapman has been involved with the evolution of the OpenMO directive-based programming standard since 2001. She also is an active participant in the OpenSHMEM and OpenACC programming standards efforts. Her work explores programming models for large-scale computing with a focus on node programming, strategies for runtime optimizations, compiler-tool interactions and high-level programming models for embedded systems.

3. REZAUL CHOWDHURY

Rezaul Chowdhury is an assistant professor in Computer Science at Stony Brook University. Prior to joining SBU he worked with the Structural Bioinformatics Group at Boston University, and the SuperTech Research Group at MIT. Before moving to Boston he was a postdoctoral fellow at the Center for Computational Visualization, Institute for Computational Engineering & Sciences at the University of Texas at Austin. He received his PhD in Computer Sciences also from UT Austin working with the Theory group. Rezaul is a recipient of an NSF Early CAREER award."

4. MARIVI FERNÁNDEZ-SERRA

Marivi Fernández-Serra is an associate professor in the Department of Physics and Astronomy at SBU. She received her PhD in 2005 from the University of Cambridge and then worked as a postdoc at the Center for Atomic and Molecular Simulations in Lyon, France. Her research is in the field of computational condensed matter physics. She develops and applies methods to study the atomic and electronic dynamics of complex materials. One of her main research areas is the study of fundamental properties of liquid water using quantum mechanical simulations. In 2010 she was awarded a DOE Early Career award to develop methods to simulate liquids under non-equilibrium conditions.

5. ROBERT HARRISON

Robert Harrison is a professor of Applied Mathematics & Statistics and the director of the Institute for Advanced Computational Science at SBU. He is also Chief Scientist for the Computational Science Initiative at Brookhaven National Laboratory. Dr. Harrison comes to Stony Brook from the University of Tennessee and Oak Ridge National Laboratory, where he was the Director of the Joint Institutes of Computational Science, Professor of Chemistry and Corporate Fellow. He has a prolific career in high-performance computing with over one hundred publications on the subject, as well as extensive service on national advisory committees.

6. XIANGMIN JIAO

Xiangmin Jiao received his B.S. in 1995 from Peking University, China, his M.S. in 1997 from University of California Santa Barbara, and his PhD in computer science in 2001 from University of Illinois at Urbana-Champaign (UIUC). After working in interdisciplinary research for a few years as a Research Scientist at the Center for Simulation of Advanced Rockets (CSAR) at UIUC and then as a Visiting Assistant Professor in College of Computing at Georgia Institute of Technology, he joined the faculty of Stony Brook University in Fall 2007. He is now an Associate Professor in the Department of Applied Mathematics and Statistics and is affiliated with the Computer Science Department.

7. MARAT KHAIROUDINOV

Marat Khairoutdinov obtained his PhD degree in 1997 from the University of Oklahoma. From there he was employed as a Research Scientist at Colorado State University and then came to Stony Brook's School of Marine and Atmospheric Sciences in 2007. During his PhD studies, he developed one of the first Large Eddy Simulation (LES) models with explicit/bin microphysics and applied it to study the evolution of drizzling marine stratocumulus clouds. After graduating, he redesigned his LES model to handle deep convective clouds and made it suitable to run on massively parallel computers. The new cloud-resolving model named System for Atmospheric Modeling, or SAM, has been applied to various interesting convection problems and is being used by scientists in their research at a wide variety of institutions.

8. PREDRAG KRSTIC

Predrag Krstic is a Research Professor at the Institute for Advanced Computational Science and founder and owner of the Theoretik consulting. He was a member of the senior research staff in the Physics Division at Oak Ridge National Laboratory (1995-2011). His research covers a wide range of fields in theoretical atomic physics, plasma physics and nuclear fusion, computational physics and chemistry, plasma-surface interactions, molecular electronics, and bio nanotechnology. His work has been disseminated in more than 200 papers in peer-reviewed journals, in several patents, and in book chapters. He is the editor of a number of conference proceedings, a member of editorial boards and advisory committees, a consultant of the International Atomic Energy agency, and elected Fellow of the American Physical Society.

9. ARTEM OGANOV

Artem Oganov received his PhD in Crystallography from the University College London in 2002. He was a Group Leader at ETH Zurich from 2003-2008, at which time he came to Stony Brook as an Associate Professor and then became a full professor in 2010. His career record boasts over 122 papers published, one book, 2 patents, and he has given over 200 talks and colloquia. Professor Oganov is on the Editorial Board member of the "Journal of Superhard Materials" and "Scientific Reports" (Nature Publishing Group), he has refereed for more than 60 journals and for Oxford University Press book publishing, and he is the founder and chairman of the Commission on Crystallography of Materials (International Union of Crystallography). Most recently he has become the Director of the Center for Materials by Design at Stony Brook University.

10. MATTHEW REUTER

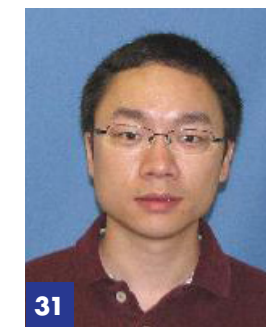
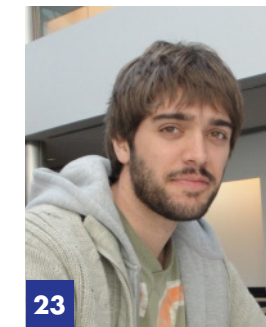
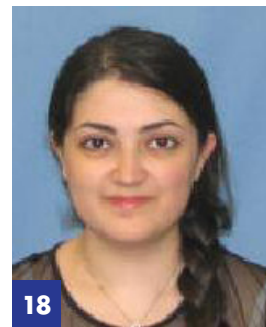
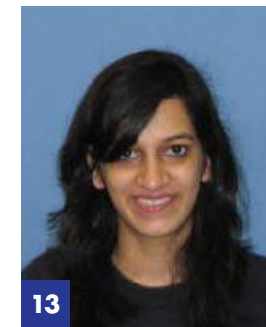
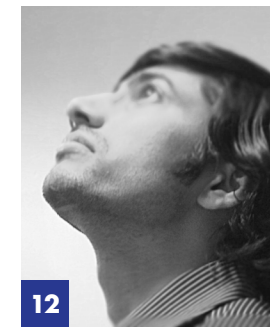
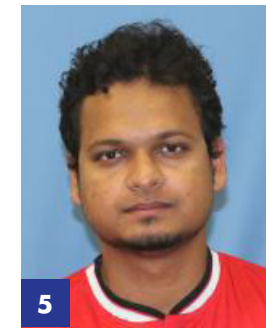
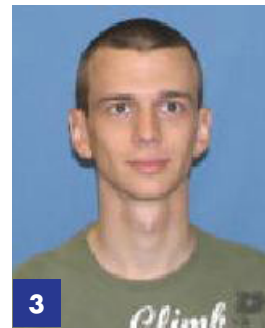
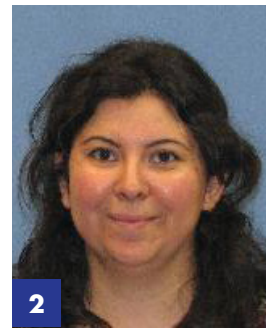
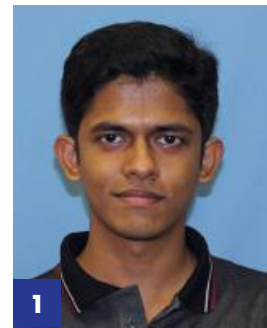
Matt Reuter joined SBU in 2015 as an Assistant Professor. Prior to coming to Stony Brook he was a Research Associate in the Department of Chemistry at Northwestern University, where he studied single-molecule behavior. He received B.Sc. degrees in chemistry and mathematics from Michigan Technological University (2006) and a PhD degree in theoretical/ computational chemistry from Northwestern University (2011). From 2011 to 2013, he was a Eugene P. Wigner Fellow at Oak Ridge National Laboratory, where he developed theories and algorithms for studying electron transport processes and materials chemistry. Matt is the lead author of more than 20 peer-reviewed journal articles. He was also the recipient of a U.S. DoE Computational Science Graduate Fellowship for most of his graduate studies at Northwestern.

11. ARNOUT VAN DE RIJT

Arnout van de Rijt received his PhD from Cornell University. He came to the Sociology Department at Stony Brook University in 2007, and in 2013 he was granted tenure. His research interests include Social Networks, Collective Action, Cumulative Advantage, Mathematical Sociology, and Computational Methods. For his contributions to social network analysis he received the 2010 Freeman Award for Distinguished Junior Scholarship and several best article awards. His research is supported by the National Science Foundation and has been published in American Sociological Review and American Journal of Sociology, and PNAS.

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