2015 ANNUAL REPORT

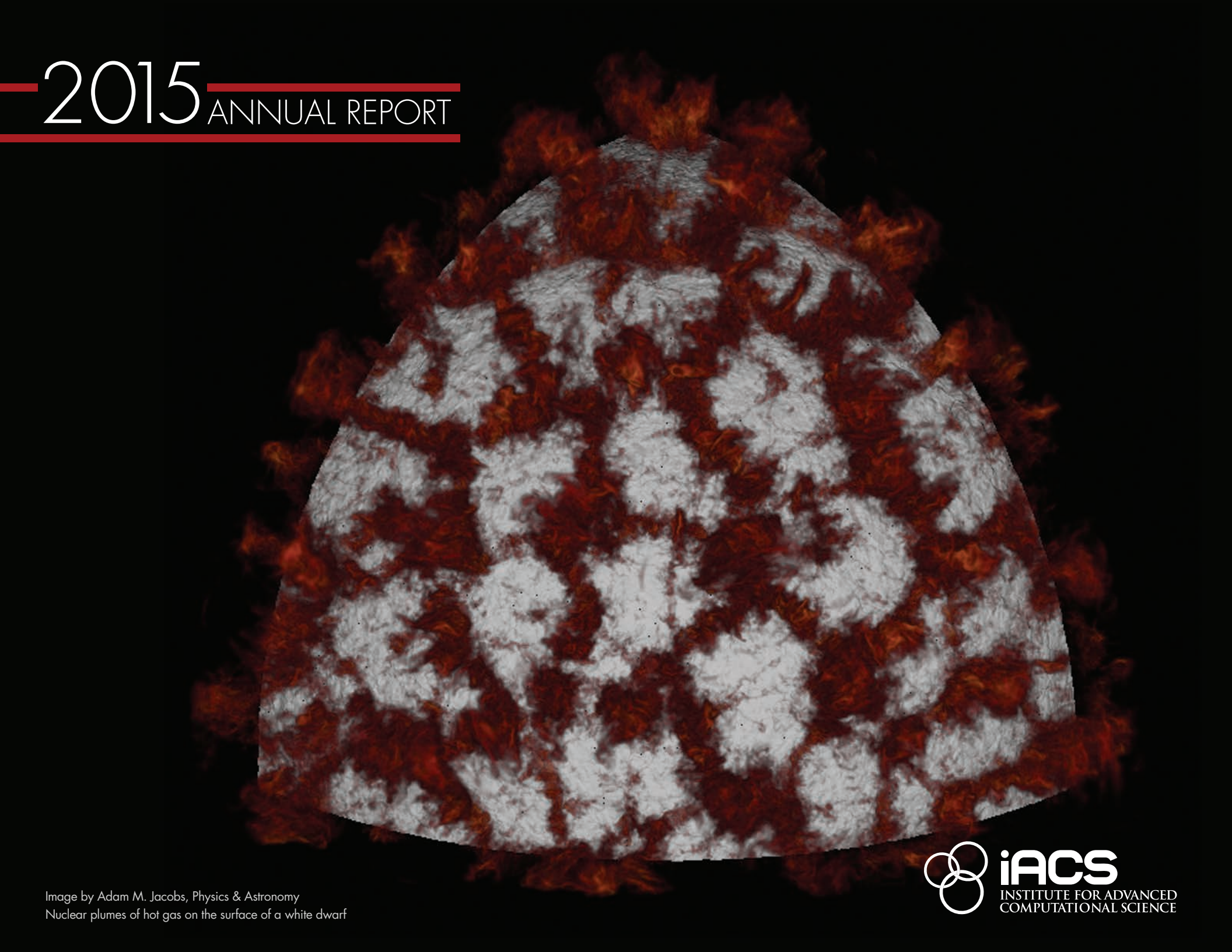

Image by Adam M. Jacobs, Physics & Astronomy
Nuclear plumes of hot gas on the surface of a white dwarf

iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

MESSAGE FROM THE DIRECTORS


IACS Director Robert Harrison and Deputy Director Alan Calder

Dear Friends and Colleagues,

Our third full year here at IACS has been monumentally successful on many fronts, and we would like to share with you some of the highlights as well as communicate our great enthusiasm and excitement. Prof. Alan Calder has agreed to serve as the IACS Deputy Director for a 3-year term. Alan brings his experience, thoughtful approach, and computational prowess (a winner of the SC2000 Gordon Bell Prize) to benefit IACS and indeed all of Stony Brook. Already he has been instrumental in putting together the proposed advanced graduate Certificate in Data and Computation in Science and Engineering (CDCSE), which is now in Albany for review. We expect final approval shortly and hope to enroll our first cohort of students in Fall 2016.

CDCSE is a wonderful illustration of the multidisciplinary spirit and plans of IACS: The certificate serves all of SBU and includes 96 courses from many departments including Physics, Applied Mathematics & Statistics (AMS), SoMAS, Sociology, Computer Science (CS) and Materials Science & Engineering (with Ecology and Evolution, Linguistics, and others poised to being added). As further testament to our multidisciplinarity, we were recently awarded a $1.4M grant from the National Science Foundation that was matched by $300K from NYS and $300K from internal SBU sources, totaling $2M for the purchase of a third high-performance cluster that will replace the original SeaWulf. This new system will be used, at a minimum, by faculty and students in 13 different departments ranging from Anatomical Sciences to Sociology.

Of special note this year was our grand opening ceremony in September, led by SBU President Samuel Stanley, New York State Assemblyman Steven Englebright, and SBU Provost Dennis Assanis, with over 150 people in attendance. This made official our move from our temporary home to our new IACS building (see page 8).

As we've written before, it is our excellent faculty, students and staff that define us, and this past year we brought Prof. Barbara Chapman on board (see page 4). She is a core IACS faculty member with a shared appointment in AMS and CS and a joint appointment with Brookhaven National Laboratory. Barbara brought with her Research Assistant Professor Dounia Khaldi, who has been involved in developing parallel intermediate representation of compilers for optimizing PGAS programs.

A third hire this year was Sarena Romano as our Travel and Event Coordinator. Sarena is brilliant at arranging visitors' travel, organizing our many events and making visitors feel welcome and at ease so they can focus on successful collaborations with our faculty and students. We also added nine new affiliate faculty for a total of 31, and 20 new students for a total of 125. The new departments and/or institutions involved are: Linguistics, Music, Chemistry, SoMAS, Toyohashi University, Nagoya University and The College of New Rochelle (see page 5).

2015 was also a year of firsts for us: We held our first high school summer camp, IACS Computes! We also held our first IACS Advisory Board meeting, and we are very grateful to the board members for their time and effort as well as their very thoughtful and valuable consideration. Late in the year our graduate students formed the new IACS Student Association made up of students from Mechanical Engineering, AMS and CS, and for the first time awards were given to two IACS New Recruits (page 12) along with four IACS Junior Researchers for a total of $59K expended on recruiting new stellar talent as well as reinforcing our commitment to the excellent research being performed by our more senior students.

Our pursuit of external funding continued this year with 22 proposals submitted for a total of $67,962,426: Eight proposals are still pending (valued at $57,744,628) and ten were awarded (valued at $5,702,131). In addition, IACS installed (noting the hard work of Firat Coskun and strong support from DoIT staff) the new $1M, 100-node, high-performance cluster (LI-red) which provides computational services to the entire campus community as well as to our NYS industrial partners and has over 150 active users.

IACS is very grateful to many people, especially our generous endowers and the SBU university leadership, specifically President Stanley, Provost Assanis and former Dean Shamash who have been steadfast in their support of our events, opportunity hires and overall mission. We must again thank the faculty and department chairs, notably Professors Arie Kaufman (CS) and Joe Mitchell (AMS), for their continued support of our hiring plans, and we welcome and look forward to working with two deans who are new to SBU, Dr. Fotis Sotiropoulos in the College of Engineering and Applied Sciences and Dr. Sacha Kopp in the College of Arts and Sciences.

This year we would also like to thank Vice Provost for Graduate Education and Graduate School Dean Charles Taber, Associate Provost for Integration of Research, Education and Professional Development Nancy Goroff, and all the members of the Graduate Council for their careful and constructive consideration of our certificate application. We would also like to make a special call out to Former Assistant Dean for Diversity and Director of the Center for Inclusive Education Nina Maung-Gaona for her tireless efforts in helping us work to increase and support diversity in our ranks as well as in submitting proposals for graduate training grants.

And finally, on behalf of all the faculty, students and staff in any way associated with IACS we would like to recognize and thank the IACS Administrative Director, Lynn Allopenna who truly has been central and tireless in not just making nearly everything happen but in leading many of our initiatives. None of our accomplishments this year would have been possible without the selfless contributions from those mentioned here as well as from many unnamed participants, to whom we are indebted.

Yours sincerely,

OUR MISSION

To realize our vision, IACS will make sustained advances in the fundamental techniques of computation and data, with high-impact applications in engineering and the physical, environmental, life and social sciences. Emphasizing excellence and diversity in our actions, we will grow to ~150 people by 2018. In coordination with the Center for Data Driven Discovery at Brookhaven National Laboratory, our dynamic and diverse institute will serve as an ideal training and proving ground for new generations of students and researchers, and will provide computational leadership and resources across the SBU campus and the State of New York.

OUR 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.

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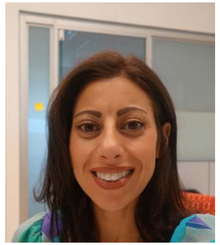
NEW HIRES



Sarena Romano
Travel and Event Coordinator

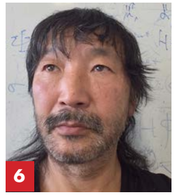
Sarena Romano was hired in May 2015 as the Travel and Event Coordinator for the institute. She has worked at Stony Brook since 2012. Her prior positon at SBU was Executive Assistant to the director of the Center for Thermal Spray Research which included the planning and coordination of two annual consortium events both on and off campus. Prior to her hire at SBU, Sarena worked as a Customer Service Manager at Tanger Outlets in Deer Park, NY as well as a new home designer for a prominent home builder in New Jersey.

Dounia Khaldi
Research Assistant Professor

Dr. Khaldi joined SBU in November 2015 as an IACS Research Assistant Professor. Dounia Khaldi was a post-doctoral researcher with the HPCTools group at the University of Houston. In her previous role at UH, she was involved in developing parallel intermediate representation of compilers for optimizing PGAS programs; specifically, she was leading the OpenSHMEM analyzer tool project in LLVM compiler. Dr. Khaldi also leads an effort to adapt the implementation of OpenMP to minimize data motion across the entire computing system and participates in educational activities, elaboration and leading several granted projects from NSF, DOE as well as industry such as Intel and AMD.
Before joining the University of Houston, Dounia Khaldi received a PhD degree with honors at MINES ParisTech school in France in 2013. Her thesis work was focused on the automatic task parallelization of sequential programs. She was granted a Master Recherche, majoring in HPC (High Performance Computing), by the Université de Versailles Saint-Quentin-en-Yvelines, France in 2010.

Barbara Chapman
Professor

Dr. 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 Ph.D. 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 OpenMP 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.



NEW AFFILIATES

1 Thomas Graf
Assistant Professor
Linguistics
Stony Brook University

2 Stephan Irle
Professor
Nagoya University

3 Dima Kozakov
Assistant Professor
Applied Math & Statistics
Stony Brook University

4 Dimitris Samaras
Associate Professor
Computer Science
Stony Brook University

5 Meg Schedel
Associate Professor
Music
Stony Brook University

6 Hideo Sekino
Professor
Computer Science & Engineering
Toyohashi University of Technology

7 Fotis Sotiropoulos
Dean
College of Engineering
& Applied Sciences
Stony Brook University

8 Lee Warren
Assistant Professor
Chemistry
The College of New Rochelle

9 Song Wu
Assistant Professor
Applied Math & Statistics
Stony Brook University

10 Minghua Zhang
Dean
School of Marine & Atmospheric Sciences
Stony Brook University

11 Wei Zhu
Professor
Applied Math & Statistics
Stony Brook University

IACS SEMINAR SERIES

February 5, 2015
Yuan Tang, Software School, Fudan University, Shanghai, China
Cache-Oblivious Wavefront: Improving Parallelism of Recursive Dynamic Programming Algorithms without Losing Cache-Efficiency

February 26, 2015
Barry Schneider, NIST
Novel Numerical Methods for the Solution of the Time Dependent Schrödinger Equation

March 5, 2015
Tim Lance, NYSERNet
The Illusion of Managing Big Data and Big Computation

April 2, 2015
Phillip Colella, Lawrence Berkeley National Laboratory
Tradeoffs in the Design of High-Performance Computational Simulations in Science and Engineering

April 9, 2015
Kerstin Lehnert, Columbia University
Making Small Data BIG: Insights from a Long-tail Geoscience Domain

April 16, 2015
Haibin Su, Nanyang Technological University
Multi-Paradigm Simulations at the Nanoscale: Methodology & Applications to Functional Carbon Materials

June 26, 2015
Chandrajit Bajaj, University of Texas at Austin
Low Discrepancy Samplings of High Dimensional Geometric Spaces with Applications

August 27, 2015
Marek Michalewicz, A*STAR Singapore
Infinicortex: Another Path to Reach Exascale Supercomputing

October 8, 2015
Heather Lynch, Stony Brook University
Satellites, Software, and Polar Cyberinfrastructure: Creating a Data-to-Information Pipeline for Antarctic Science

October 15, 2015
Shinjae Yoo, Brookhaven National Laboratory
Unsupervised Learning on Scientific Data

October 22, 2015
Alexander Turbiner, Nuclear Science Institute, UNAM, Mexico
Quantum 3-body Coulomb Problem: A Numerical Challenge

October 29, 2015
Barbara Chapman, Stony Brook University
Directive-Based Parallel Programming at Scale

November 4, 2015
Udo von Toussaint, Max-Planck-Institute for Plasmaphysics, Germany
Steel as an Option for a Plasma-facing Material at the Main Chamber Wall of a Fusion Reactor

November 5, 2015
Margaret Schedel, Stony Brook University
The Data Sensorium: Multimodal Exploration of Scientific Data Sets

November 12, 2015
Jason Jones, Stony Brook University
Multi-Million Subject Experiments in Political Mobilization

December 3, 2015
Renata Wentzcovitch, University of Minnesota
Modeling Earth's Interior from Atomic to Global Scale

PROJECTS, PROGRAMS & EVENTS

January 22-23, 2015
Intro to Python
Stony Brook University

May 5, 2015
Networking Social
Bliss Restaurant

June 25, 2015
Introduction to Parallel Programming Using OpenMP
Stony Brook University

July 13-17, 2015
IACS Computes! HS Summer Camp
Stony Brook University

August 2, 2015
New York Scientific Data Summit
New York University

August 17-21, 2015
Developing Models for Structure and Style in Scientific Writing
Stony Brook University

September 11, 2015
1st Annual Apps & Ale Social
Stony Brook University

September 18, 2015
IACS Grand Opening Ceremony
Stony Brook University

November 7-9, 2015
Sensitivity, Error and Uncertainty Quantification for Atomic, Plasma and Material Data
Stony Brook University

November 19, 2015
Etiquette Dinner
Stony Brook University

December 3, 2015
IACS Student Association Kickoff Event
The Bench Bar & Grill

Stony Brook University held a grand opening for the Institute for Advanced Computational Science (IACS). Cutting the ribbon, in center, are Samuel L. Stanley Jr., MD, Stony Brook University President, and Robert Harrison, IACS Director. Also pictured, from left: Alan Calder, Mary Hall, Wolfgang Wander, Steve Englebright, Lynn Allopenna, Dennis Assanis, Peter Paul, and Margaret Wright.

STONY BROOK OPENS NEW $20-MILLION SUPPORTED INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

Stony Brook University held a grand opening for the Institute for Advanced Computational Science (IACS), a $20-million supported 6,000 square-foot facility with the mission to make sustained advances in the science of computation and its applications to complex problems in many fields. The IACS fosters a collaborative environment, with a vision that by 2017 it will be an internationally recognized center with research and education programs and a demonstrated economic benefit to New York State. Stony Brook University leadership, IACS faculty, students and public officials attended the event.

The establishment of the IACS was made possible by a transformational $10 million anonymous donation plus matching funds from the Simons Foundation for a total of $20 million in philanthropic support.

"The creation of the IACS is consistent with Stony Brook's mission to encourage the untethered pursuit of scientific discovery among our faculty to better understand our world and universe," said Samuel L. Stanley Jr., MD, Stony Brook University President. "The collaborative academic and industry-related work that will take place at the Institute will push and advance basic science research at Stony Brook and bring forth new ideas and breakthrough discoveries."

Supercomputers play an ever increasing role in cross-disciplinary research, and the use of high-performance computers is changing the way science gets its answers, industry develops products and society analyzes its needs. The interdisciplinary IACS, working closely with Brookhaven National Laboratory (BNL) and the Computational Science Center, will further cultivate cutting-edge academic and industry collaboration and pool the power of its computer resources together to transform research in many fields of society.

"Stony Brook is already a University that computes with over $40 million worth of federal funding that has computation data as a central element," said Dennis N. Assanis, Provost and Senior Vice President for Academic Affairs. "The IACS will broaden our use and capabilities of computational data, and it will lead campus-wide initiatives in education and research computing infrastructure."

Provost Assanis also announced the availability of a new 100-node computer cluster built within the IACS. The cluster, a set of computers connected by a super high-speed network, is a state-of-the-art high-performance system that will have greater speed, memory and computational capacities than any other previously used at the University. The new system will enable faculty, students, and engineers in industry to perform simulations and to analyze data sets at a powerful rate and level of sophistication for research in fields ranging from the physical and social sciences to biological sciences, and for commercial product development.

"Computational science, which combines the crucial discipline of simulation and the exploding discipline of 'big data,' is central to all fields of human endeavor, science, society and industry," said Robert Harrison, PhD, Professor and Director of the IACS. "This cuts across all of Stony Brook University, and I like to think of the IACS as being an institute without walls between disciplines since computational science is so multidisciplinary."

Stony Brook and Brookhaven National Laboratory obtained a $1 million grant in 2014 from the Long Island Research and Economic Development Council (LIREDC) for the purchase of the computer cluster. The grant is part of a broader initiative by Stony Brook and BNL to boost job creation throughout the entire region and state. The funding source for LIREDC is the New York State's Empire State Development program, and the IACS will receive the funds through the SUNY Research Foundation.

Assemblymen Steve Englebright congratulated Stony Brook University for having the vision to develop the IACS and called it a tremendous example of innovation, research and education for the community, Long Island and New York State.

All attending the grand opening had the opportunity to see the new computer cluster and to tour the new facility, which, incredibly, includes about 10 miles of high-speed network cables. In addition to the computer cluster, the IACS features 18 offices, a 45-seat seminar room, and state-of-the-art audiovisual systems.

Professor Harrison expects the IACS to grow considerably in the coming years. Currently, there are 11 core faculty representing a cross-disciplinary range of departments in the physical and social sciences, along with 23 associated faculty from Stony Brook and other institutions. Student research will also thrive at the IACS, as 43 core and 60 affiliate graduate students have access to IACS resources to advance their work.

1. Assistant Professor Jason Trelewicz (far left), who is the Program Director for HPC^{NY}, speaks with ceremony attendees about the success of his interdisciplinary project that links SBU research to local industry. 2. (L-R) IACS Director Robert Harrison, SBU President Samuel Stanley, SBU Provost Dennis Assanis, SBU Vice President for Economic Development Yacov Shamash and SBU's former Associate Vice President for Brookhaven Affairs Peter Paul stand in front of the newly acquired HPC Llred cluster. 3. SBU President Samuel Stanley talks with IACS PhD student Bryan Perozzi about his research. 4. SBU President Samuel Stanley addresses the crowd at the IACS Opening Ceremony. 5.SBU Provost Dennis Assanis (right) speaks with ceremony attendees. 6. IACS Director Robert Harrison (left) reviews talking points with SBU President Samuel Stanley before the opening ceremony.

WINNERS' RESEARCH RANGES FROM ANTARCTIC PENGUINS TO DARK MATTER

IACS 2015 Jr. Researcher Award winner Philip McDowall

By Erica Cirino

Most people don't associate computing with nature. Yet, as technology advances and new environmental problems arise, ecologists are increasingly turning to computing as a means of better understanding the natural world around us. One area of particular interest is animal species' geographic distribution in relation to changes in the environment. This area of research is called spatiotemporal dynamics, and it has taken Philip McDowall, one of the winners of the Institute for Advanced Computational Science (IACS) 2015 Junior Researcher Award, all the way to Antarctica.

"The area I work in, the Western Antarctic Peninsula, is one of the fastest-warming places on Earth," said McDowall, who specifically studies the distribution of three species of Antarctic penguins. "Ecologists are often interested in the relationship between environmental factors and the spatial distribution of a species or population. Understanding these associations can be vital for predicting species ranges, predicting how a species will react to climate/habitat change, and developing effective management or conservation strategies."

> "THE AREA I WORK IN, THE WESTERN ANTARCTIC PENINSULA, IS ONE OF THE FASTEST-WARMING PLACES ON EARTH"

McDowall, from the Department of Ecology and Evolution, studies with Assistant Professor Heather Lynch. For him, receiving an IACS Junior Researcher Award means not only the opportunity to use and access new technology with which he carries out his research, but also the ability to travel and network with other researchers in his field of ecology and evolution. "I'm really looking forward to having more opportunities to talk to people using computational science in other disciplines. I think there are a lot of people working on similar questions in very different systems, and there's so much to be learned from the ways other people have dealt with computationally intensive problems, so it's great to be supported by such an interdisciplinary group as the IACS."

The research presented by award applicants was of such high caliber this year that IACS granted two Jr. Researcher Awards, the second of equal value going to Adrian Soto, from the Department of Physics & Astronomy who studies with Associate Professor Marivi Fernández-Serra. Soto applies computational methods to condensed matter physics, or the science of how liquids and solids are composed on the molecular level. Specifically, Soto is interested in understanding how the interactions between water molecules cause liquid water to form—for applications like battery design—and also how liquid and solid semiconducting materials—such as silicon—can be used to detect dark matter in the universe. Being able to study diverse subjects like water, the most abundant and studied molecule on earth, and dark matter, one of the biggest mysteries of science, said Soto, proves that the potential applications for computational science are virtually endless.

"It feels great to get an official recognition to [my] hard work," said Soto. "This award is going to allow me to attend conferences and schools, where I will explain my research and learn from others. I know of many people who met their next employer at a science conference. Why couldn't that happen to me?"

The awards are for advanced PhD students who use computational science in their research with IACS faculty. It raises winners' regular stipends to $34,000 for up to three years and also provides winners with $4,000 per year for travel to PhD-related conferences and events.

These awards and the formation of IACS were made possible by an anonymous donation of $10M matched by another $10M from the Simons Foundation. The Institute provides resources for and engages with faculty, students and postdocs from a wide variety of academic backgrounds, all who have research interests that involve the use of high-performance and data-intensive computing.

IACS 2015 Jr. Researcher Award winner Adrian Soto

TWO NEW RECRUITS JOIN IACS AND RECEIVE AWARDS FOR FALL 2015

Alex Borowicz will pursue a PhD in Ecology & Evolution; DW Han, a PhD in Physics & Astronomy

By Erica Cirino

Each year IACS awards its New Recruit Award to "stellar," new incoming graduate students who plan to undertake research related to computational science. The awards provide support, primarily in the forms of funding and mentorship, so that high-potential students can thrive in their studies at Stony Brook University.

Recently, IACS announced the recipients of the new recruit award for Fall 2015. The two students, who will both be pursuing doctoral degrees, are Alex Borowicz and Dongwon (DW) Han. The award is in addition to their regular stipends provided by their home departments and raises their stipends to $32,000 for 1 calendar year, plus $4000 for travel and equipment. IACS awardees are permanently identified on the IACS website and in IACS publications, and their work will be highlighted in IACS workshop and conference proceedings.

DW Han

Accepted into the Physics and Astronomy PhD program, Han has yet to choose his IACS-affiliated mentor. "I have not decided my research topic, but I know that my research will involve analyzing large and complex data."

Han moved to the United States from South Korea 10 years ago. He earned his BS in Mathematics, with minors in Computer Science and Physics, from the University of Massachusetts Amherst in 2013, and he has been working as a software developer in Waltham, Massachusetts since graduation. Han said that pursuing his doctorate at Stony Brook would provide him with a means of transitioning out of a job in industry to a research-based career in a national laboratory. Han said he believes that the same "big data" computing used by high-tech industry companies to better understand their ever-growing data sets "can be readily applied to analysis of complex physical systems" in the fields of physics and astronomy, which are fields producing data that have historically been analyzed using statistics.

Receiving the award was humbling, said Han, adding that he is "thankful" for the support - financially and otherwise - afforded to him by the IACS New Recruit Award, which he said will help him facilitate his research and further his education.

For more information about the resources and opportunities available to students and faculty through the Institute for Advanced Computational Science, visit www.iacs@stonybrook.edu.

Alex Borowicz

Accepted into the Ecology and Evolution PhD program, Borowicz will be working with IACS Affiliate Assistant Professor Heather Lynch. Borowicz said that he was "thrilled" to be offered the award, especially because it would afford him the opportunity to execute research projects incorporating computation, an area which he said is a bit outside of his typical research comfort zone. "I was trained in more of a natural history approach to ecology that emphasized observation and careful thought," said Borowicz. "Obviously in order to produce meaningful results, ecology does need to be a quantitative science, so I'm really looking forward to bringing the natural history tradition into quantitative ecology that's at the heart of Heather's lab."

Borowicz earned his BA in Human Ecology from College of the Atlantic in Bar Harbor, Maine in 2014. Over the years he has amassed a great deal of hands-on experience in the field of wildlife science, working at the Wild Spirit Wolf Sanctuary in New Mexico and then in the Gulf of Maine studying seals and whales. At Stony Brook, he said he plans on studying the impacts of climate change on Antarctic organisms and ecosystems. Specifically Borowicz said that he seeks to study marine mammals and "seals in particular, to examine both the population dynamics of the several species in the region and the ways in which physical changes affect how they manage life in a challenging environment."

HPC NY

HIGH PERFORMANCE COMPUTING CONSORTIUM

HPC^{NY} Director Jason Trelewicz

The New York State High Performance Computing Consortium (HPC^{NY}) is a NYSTAR funded program that unites computing expertise from the Institute for Advanced Computational Science (IACS) at Stony Brook University (SBU), Rensselaer Polytechnic Institute, the Center for Computational Research at SUNY Buffalo, the Mount Sinai School of Medicine, and Marist College. The mission of HPC^{NY} is to engage New York State companies on the use of high performance computing and data analytics for achieving a competitive advantage in advanced manufacturing and technology industries. This past year has included the launch of a new website (https://hpc-ny.org/) to facilitate the expansion of industrial engagements across the state. At SBU, we have had a particularly exciting year that included the addition of two new HPC^{NY} projects, the forging of new collaborations with the Centers for Advanced Technology in Integrated Electric Energy Systems and Diagnostic Tools and Sensor Systems, and many individual achievements across our entire project portfolio.

The HPC^{NY} team at SBU has grown to encompass six projects with faculty members representing departments in the College of Engineering and Applied Sciences as well as the College of Arts and Sciences. Of the two new projects added to the HPC^{NY} portfolio, the first is under the direction of Professor Dilip Gersappe of the Materials Science and Engineering Department (MSE) and is a collaboration with EOS Energy Systems. The focus of this project is on developing Lattice-Boltzmann models to simulate and optimize zinc/bromine batteries for grid storage applications. The second project is a partnership with Absara Audio led by Professor Yuefan Deng in the Department of Applied Mathematics and Statistics (AMS) in collaboration with Professor Margaret Schedel of the Department of Music. This exciting new endeavor, which involves a unique industry in the HPC^{NY} portfolio, is combining parallel computing techniques with machine learning algorithms to analyze the frequency spectra of musical instruments to support the development of groundbreaking digital audio products.

PIGTRONIX FUTURISTIC AUDIO TECHNOLOGY

Significant progress has been made on the four other projects involving a wide range of simulation methodologies from atomistic to continuum approaches working with Professors Xiangmin Jiao (AMS), T.A. Venkatesh and Jason Trelewicz (MSE), and Sotirios Mamalis (Mechanical Engineering) through partnerships with ParaLab Computing, Thermolift, TheoretiK, and Innoveering, respectively. The HPC^{NY} project with Innoveering in collaboration with Professor Mamalis has secured over $2M in federal funding to support the development of a robust catalytic reformer that can use any hydrocarbon fuel to create syngas (a mixture of CO and H2) for improving the combustion characteristics of heavy-duty engines used in stationary power generation. Dean Modroukas, Ph.D., President of Innoveering LLC, has praised the HPC^{NY} model stating that, "high performance computing and our partnership with the Institute for Advanced Computational Science at Stony Brook University is accelerating innovation and technology deployment for Innoveering. These efforts will advance the state of the art in next generation power and propulsion technology."

In closing, we would like to note that in 2015 the institute purchased a 100-node cluster, LIred, made possible with funding from the New York State's Long Island Research and Economic Development Council. This cluster is intended for use by our local industrial partners as well as other companies around the state. Potential users should contact Jason.Trelewicz@stonybrook.edu for access to and to find out about computational parameters for the LIred system.

BIG DATA RESEARCH AT STONY BROOK GETS BIG BOOST WITH NSF FUNDING FOR COMPUTER CLUSTER

Stony Brook, N.Y., November 5, 2015 – The National Science Foundation (NSF) has awarded the Stony Brook University Institute for Advanced Computational Science (IACS) a $1.4 million Major Research Instrumentation (MRI) grant to acquire an additional high-performance computer system that will further build the University's computational capacity and big data analyses in research and education initiatives encompassing all fields. Total funding for the computer cluster will reach $2 million, based on $600,000 in matching grants from internal University sources and the Empire State Development's NYSTAR program ($300,000).

To be installed during the first half of 2016, the computer cluster will replace a previous high-peformance cluster, called "SeaWulf," and be installed within the Division of Information Technology (DoIT). To date the cluster has been an important component to advancing research and education in the areas of Computer Science, Mechanical Engineering, Chemistry, Biomedical Engineering, Applied Math, Physics, Geosciences, Pharmacology and Public Health. The new SeaWulf will have 50 times the processing power of its predecessor enabling faster and more powerful analyses of huge data sets in all these fields of study and in many other disciplines. Students will acquire valuable experience using SeaWulf and build the skills they need to work in supercomputing fields such as Information Technology.

"With SeaWulf's increased computational power and speed, faculty and students will be able to input and manipulate data at the highest levels of sophistication available in computing," said Robert Harrison, PhD, Professor and Director of the IACS and Principal Investigator of the MRI grant. "The system will be another transformative technology for computing, research and educational endeavors campus-wide."

Dr. Harrison added that although the new high-performance computer cluster will primarily be used to support education and research at Stony Brook University, a portion of its capacity (up to 30 percent) will be made available for users across the SUNY educational system and regional industries. One partner with Stony Brook that will have early access to SeaWulf is the School of Arts and Sciences at the College of New Rochelle.

Stony Brook IACS Director Robert Harrison, second from right, leads the SeaWulf computer cluster initiative to further build the University's computational capacity. Also instrumental in the implementation of SeaWulf are, from left: Firat Coskun, a Senior Programmer Analyst for IACS and DoIT; Andrew White, Senior Director, Research Computing, DoIT; and Yuefan Deng, Professor of Applied Mathematics & Statistics.

The MRI grant and matching funds enables the IACS to purchase and operate SeaWulf for four years. In addition to being designed to greatly enhance the quality and functionality of the research cyber infrastructure, the highly re-configurable and extensible system will also provide significant cost savings for the University. The new system supports both sophisticated and entry-level users through command-line and web-portal access and supports cloud-based software and batch workflows. SeaWulf also provides users with a highly customizable and secure environment while facilitating overall resource management.

The computer cluster will be the second high-performance system installed by the IACS within one year. The first was completed in October 2015 and unveiled during the IACS grand opening.

WOMEN IN THE MEDIA

Mirroring a major problem in society at large, women are significantly shortchanged when it comes to media coverage, with men being mentioned in the news a whopping five times more than women. This is the major finding of a first-of-its-kind study by Stony Brook University researchers. The paper, titled "A Paper Ceiling: Explaining the Persistent Underrepresentation of Women in Printed News," is published in the American Sociological Review.

In the 21st Century women continue to receive substantially less media coverage than men, despite women's much increased participation in public life. Women are closing the gender gap in many social fields and sometimes even outperform their male counterparts, such as in college graduation rates. Yet when you read a name on a news website or hear a name on the radio, the odds are 5 to 1 that it refers to a man. Why are women muffled in the media? It's a question that social scientists have grappled with for decades.

Essentially, the researchers found the answer when they distinguished between famous individuals who appear regularly in the news and obscure individuals who make the news only once or twice. Among obscure individuals, they found near-parity, with a female name for almost every male name. Women are outnumbered only at high levels of coverage, among individuals at the top of social hierarchies, who are mostly men: CEOs, congressmen, movie directors, and the like. And because these famous individuals account for most of the name occurrences in the news, the overall coverage difference between women and men has remained so wide.

"Contrary to claims made by earlier researchers, women's coverage does not noticeably pick up when male editors are replaced by female editors," said Arnout van de Rijt, Associate Professor of Sociology and the Institute for Advanced Computational Science at Stony Brook University and co-author of the study. "This study also found women's coverage to be no greater in news produced by liberal media organizations."

An interdisciplinary faculty research team from Stony Brook University's Institute for Advanced Computational Science used high performance computing methods to assess that women are significantly underrepresented in media coverage. From left: Arnout van de Rijt, Vivek Kulkarni, and Steven Skiena. Using high-performance computing, social and computer scientists prove gender-bias in the news in first-of-its-kind study

Stony Brook University researchers used a unique news data analysis system involving computational science that led them to their findings. The system was developed by Steven Skiena, Professor of Computer Science at Stony Brook University. Professor Skiena and graduate student Vivek Kulkarni, both co-authors of the study, used this system to aggregate the millions of occurrences of female and male names across scanned issues and digital records of thousands of newspapers, magazines and online news sources between 1983 and 2009, breaking these down by newspaper section, slant and organizational gender make-up.

Based on this research method and the overall findings, Van de Rijt concludes that "the persistent gender gap in media coverage is thus produced by a toxic mix of two ingredients: (1) the obsession of media with leaders at the expense of everyone else, and (2) the well-known 'glass ceiling' that continues to block off working women's access to leadership positions."

Stony Brook University collaborators on the project with Professor van de Rijt include Vivek Kulkarni, a PhD student in the Department of Computer Science; and Steven Skiena, Distinguished Professor in the Department of Computer Science.

AWARDS

Jr. Researcher Award
– Bryan Perozzi, Computer Science – Skiena
– Adam Jacobs, Physics – Zingale, Calder
– Philip McDowell, Ecology & Evolution – Lynch
– Adrian Soto, Physics – Fernandez-Serra

New Recruit Award
– Alexander Borowicz – Ecology & Evolution
– Dongwon Han – Physics

Travel Award
– Na Zhang, AMS – Deng
– Tan Li, BNL – Yu
– Cheng Chang, BNL – Yu

Young Writers Award
– Aimilios Sofianopoulos, Mechanical Engineering – Mamalis
– Xinglin Zhao, Applied Math & Statistics – Jiao

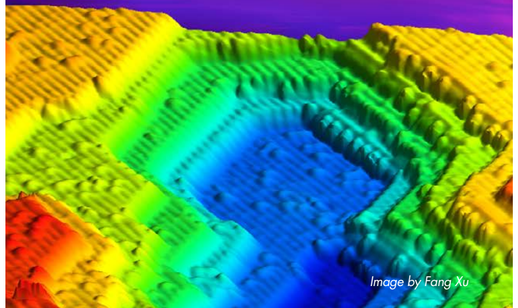


Image by Fang Xu

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ADVISORY BOARD

Mary Hall
Professor

Mary Hall is a Professor in the School of Computing at the University of Utah, where she has been since 2008. She conducts research in programming language and compiler technology for parallel and high-performance computing architectures. Her current research focuses on automatic performance tuning of scientific and data analytics applications, which involves close collaboration with architects, computational scientists and domain scientists. She has served as a member of the ACM History Committee for the past decade and chair from 2009-2013. She has also served IEEE as a member of the Computer Society Award Committee, chair of the ACM/IEEE Kennedy Award Committee, and member of the Cray and Fernbach Award Committees. She has co-authored numerous reports for government agencies, particularly NSF, DOE and DARPA, to establish the research agenda in compilers and high-performance computing. Professor Hall is an ACM Distinguished Scientist. She currently serves as ACM's representative on the Computing Research Association Board of Directors. She received an M.S. and Ph.D. in Computer Science from Rice University in 1989 and 1991, respectively, and graduated Magna Cum Laude in 1985 with a B.A. in Computer Science and Mathematical Sciences also from Rice University. Prior to joining Utah, Professor Hall was jointly a research associate professor and project leader at the University of Southern California, and previously held research positions at Caltech, Stanford and Rice.

Michael Macy
Professor

Michael Macy grew up in Tennessee but left to attend Harvard, where he received his B.A. and later his Ph.D. along with an M.A. from Stanford. He is currently a Goldwin Smith Professor of Arts and Sciences in Sociology and Director of the Social Dynamics Laboratory at Cornell, where he has worked since 1997. With support from the National Science Foundation, the Department of Defense, and Google , his research team has used computational models, online laboratory experiments, and digital traces of device-mediated interaction to explore familiar but enigmatic social patterns, such as circadian rhythms, the emergence and collapse of fads, the spread of self-destructive behaviors, cooperation in social dilemmas, the critical mass in collective action, the spread of highthreshold contagions on small-world networks, the polarization of opinion, segregation of neighborhoods, and assimilation of minority cultures. Recent research uses 509 million Twitter messages to track diurnal and seasonal mood changes in 54 countries, and telephone logs for 12B calls in the UK to measure the economic correlates of network structure. His research has been published in leading journals, including Science, PNAS, American Journal of Sociology, American Sociological Review, and Annual Review of Sociology.

Wolfgang Wander

Wolfgang Wander received his Ph.D. in High-Energy-Physics from the University of Erlangen-Nürnberg, Germany in 1996. He then became the software coordinator for the Hermes Experiment, an international High-Energy-Physics experiment at DESY, Hamburg, Germany. There he designed and operated the first PC based Linux cluster in High-Energy-Physics which was used for computationally intensive Monte Carlo simulations and the data-production of the experiment. In 1997 he became a Research Associate as Scientific Computing Facility Manager at MIT's Lab for Nuclear Science. Since 1998 Wolfgang Wander has been a member of the technical staff at Renaissance Technologies LLC in East Setauket, NY.

Margaret Wright
Professor

Margaret H. Wright received her B.S. in Mathematics, and M.S. and Ph.D. in Computer Science from Stanford University. Her research interests include optimization, linear algebra, numerical analysis, scientific computing, and scientific and engineering applications. She is Editor-in-Chief of SIAM Review and an associate editor of Mathematical Programming, the SIAM Journal on Scientific Computing, the SIAM Journal on Optimization, and IEEE Computing in Science and Engineering. She is the co-author (with Philip Gill and Walter Murray) of two books, Practical Optimization and Numerical Linear Algebra and Optimization.

Lois McInnes
Computational Scientist

Lois Curfman McInnes is a computational scientist. Her research focuses on numerical algorithms and software for the parallel solution of large-scale scientific applications involving nonlinear partial differential equations and related optimization problems. In particular, she develops such software tools within the PETSc and TAO libraries. McInnes received a PhD in Applied Mathematics from the University of Virginia in 1993. She is the winner of the 2011 Ernest Orlando Lawrence Award for outstanding contributions in research and development supporting the Department of Energy and its missions.

ADVISORY BOARD

David Keyes
Professor

David Keyes is a Professor of Applied Mathematics and Computational Science and the Director of the Extreme Computing Research Center, having served as the Dean of the Division of Mathematical and Computer Sciences and Engineering at KAUST for its first 3.5 years. Also an Adjunct Professor and former Fu Foundation Chair Professor in Applied Physics and Applied Mathematics at Columbia University, and an affiliate of several laboratories of the U.S. Department of Energy, Keyes graduated in Aerospace and Mechanical Sciences from Princeton in 1978 and earned a doctorate in Applied Mathematics from Harvard in 1984. Before joining KAUST among the founding faculty, he led scalable solver software projects in the ASCI and SciDAC programs of the U.S. Department of Energy.

Angela Violi
Professor

Angela Violi joined the faculty at the University of Michigan in 2006 as an Assistant Professor and became an Associate Professor with tenure in 2009. From 2002 to 2006 she was a Research Associate in the US Department of Energy-funded CSAFE program at the University of Utah and a Research Assistant Professor in the Chemistry Department at the University of Utah from 2004 to 2006. Her research interest is in multiscale processes occurring in reactive systems, with applications crosscutting combustion, nanoscience and biology. Prof. Violi has pioneered the use of atomistic computational models for bridging the time scales in the growth of carbon nanoclusters within the combustion environment. This work has shed new light on nanoparticle formation in high-temperature, chemically reacting flows. Prof. Violi has published approximately 50 peer-reviewed articles, and has 30 invited presentations at the national and international level. She has received multiple recognitions for her accomplishments, among them the NSF CAREER award and the international Bernard Lewis Award from the Combustion Institute for "High quality research in combustion."

THANK YOU

We want to thank our supporters and our generous donors, $10M from an anonymous source matched by $10M from the Simons Foundation, for helping us to achieve many of our goals and for providing continued support as we invest in the future. As a direct result of being supported by our endowment in 2015, we were able to accomplish the following:

- *Supported travel for 14 national and international visitors to the institute*
- *Featured 16 speakers in our IACS Seminar Series from diverse departments: Molecular Physics, Geochemistry, Computer Science, Applied Math, Ecology & Evolution, Music, Sociology, Materials Science, Engineering, Quantum Mechanics*
- *Started the IACS Student Association which held its first, student-run event this past November (30 attendees)*
- *Held two 1-day graduate student workshops (24 & 35 registrants); one 1-week high school computing camp (10 participants island-wide); one 1-week scientific writing course (15 attendees); and one 2.5-day faculty conference (40 participants nationwide)*
- *Held 5 social events: Graduate Student Networking Social (20 attendees), Apps and Ale (50 attendees); IACS Opening Ceremony (~100 attendees); Etiquette Dinner (20 attendees); and IACS Annual Anniversary Dinner (70 attendees)*
- *Awarded 4 Junior Researcher Awards; 2 New Recruit Awards; 2 Young Writers Awards; and 3 Travel Awards*
- *Hired a staff administrator, supported a new Assistant Professor and 50% of a systems administrator*
- *Supported start-up for an Assistant Professor and a Research Professor*
- *Funded $10K to the Center for Inclusive Education to help defray costs associated with increasing the participation of underrepresented minorities in the STEM fields*
- *Collaborated, trained and supported 1 high school and 3 graduate interns*
- *Provided supplies for our new state-of-the-art offices*
- *Sponsored our first Advisory Board meeting*

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

- *Recruit two endowed chairs*
- *Hire a half-time Recruiter dedicated to increasing the participation of underrepresented minorities in the STEM fields*
- *Hire a second Systems Administrator*
- *Receive approval for our 17-credit graduate Certificate in Computation and Data in Science and Engineering (CDCSE) which includes two new graduate level, computational courses*
- *Purchase and bring online a 165-node high-performance computing system*
- *Continue to build a world-class computational infrastructure with technical support to free faculty and students to focus on creativity and innovation*

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FACULTY


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1 Alan C. Calder Associate Professor and Deputy Director

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. Prior to coming to Stony Brook, he had research appointments at the National Center for Supercomputing Applications and the University of Chicago. His research is principally in bright stellar explosions known as Type Ia supernovae. The light curves of these events can be standardized and thereby used as distance indicators for cosmology studies investigating the expansion history of the Universe.

2 Rezaul Alam Chowdhury Assistant Professor

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.

3 Marivi Fernandez-Serra Associate Professor

Marivi Fernandez-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.

4 Robert J. Harrison Professor and Director

Robert Harrison is a professor of Applied Math and the director of the Institute for Advanced Computational Science at SBU. He is also the head of the Computational Science Center at BNL. Dr. Harrison comes to Stony Brook from the University of Tennessee and Oak Ridge National Laboratory, where he was the Director of the Joint Institute 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.

5 Xiangmin Jiao Associate Professor

Dr. Jiao received his B.S. in 1995 from Peking University, China, his M.S. in 1997 from University of California Santa Barbara, and his Ph.D. 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.

6 Marat Khairoutdinov Associate Professor

Associate Professor Marat Khairoutdinov obtained his Ph.D. degree in 1997 from the University of Oklahoma. From there he was employed as a Research Scientist at Colorado State and then came to SBU's School of Marine and Atmospheric Sciences in 2007. During his Ph.D. studies, he developed one of the first Large-Eddy Simulation (LES) models with explicit/bin microphysics. 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, is being used by scientists in their research at a wide variety of institutions.

7 Predrag Krstic Research Professor

Dr. Predrag Krstic is a Research Professor at the Institute for Advanced Computational Science and founder and owner of 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, laser 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.

8 Artem R. Oganov Professor

Professor 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.

9 Matt Reuter Assistant Professor

Matt Reuter joined SBU in 2014 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 Ph.D. 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 17 peer-reviewed journal articles. He was also the recipient of a U.S. DoE Computational Science Graduate Award for most of his graduate studies at Northwestern.

10 Arnout van de Rijt Associate Professor

Associate Professor 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.

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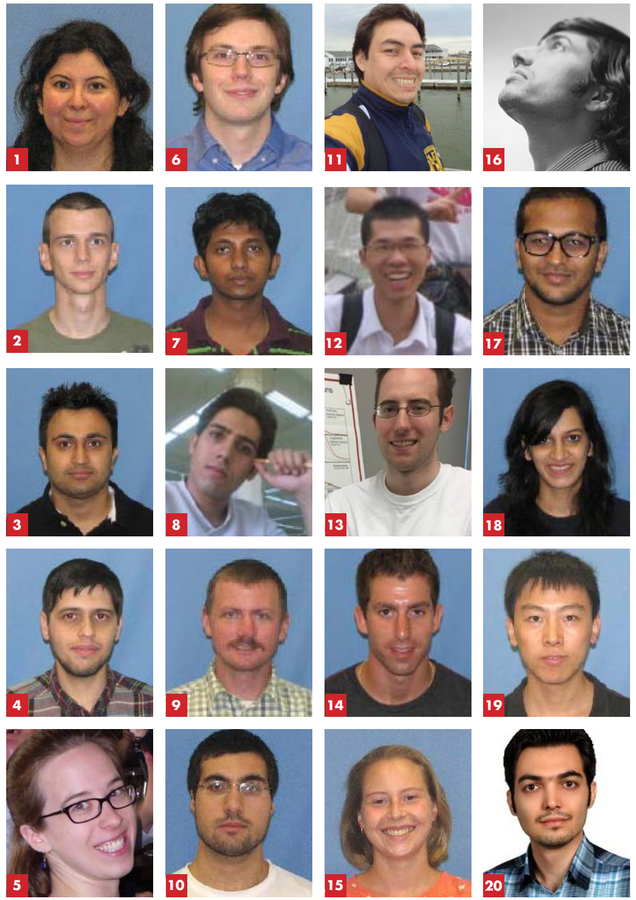
26 Yue Liu
27 Cao Lu
28 Prayag Chandran Nirmala
29 Sridhar Periasami
30 Ouutong Trump Phooprasert
31 Guangrui Qian
32 Maksim Rakitin
33 Panu Sam-Ang
34 Hyang-Gi Song
35 Adrian Soto
36 Bryan Sundahl
37 Jesmin Jahan Tithi
38 Akhil Tiwari
39 Xuebin Wang
40 Shengnan Wang
41 Donald Willcox
42 Hongfei Xu
43 Jianjin Xu
44 Oliver Yang
45 Wei Zhang
46 Xinglin Zhao
47 Xin Zhou



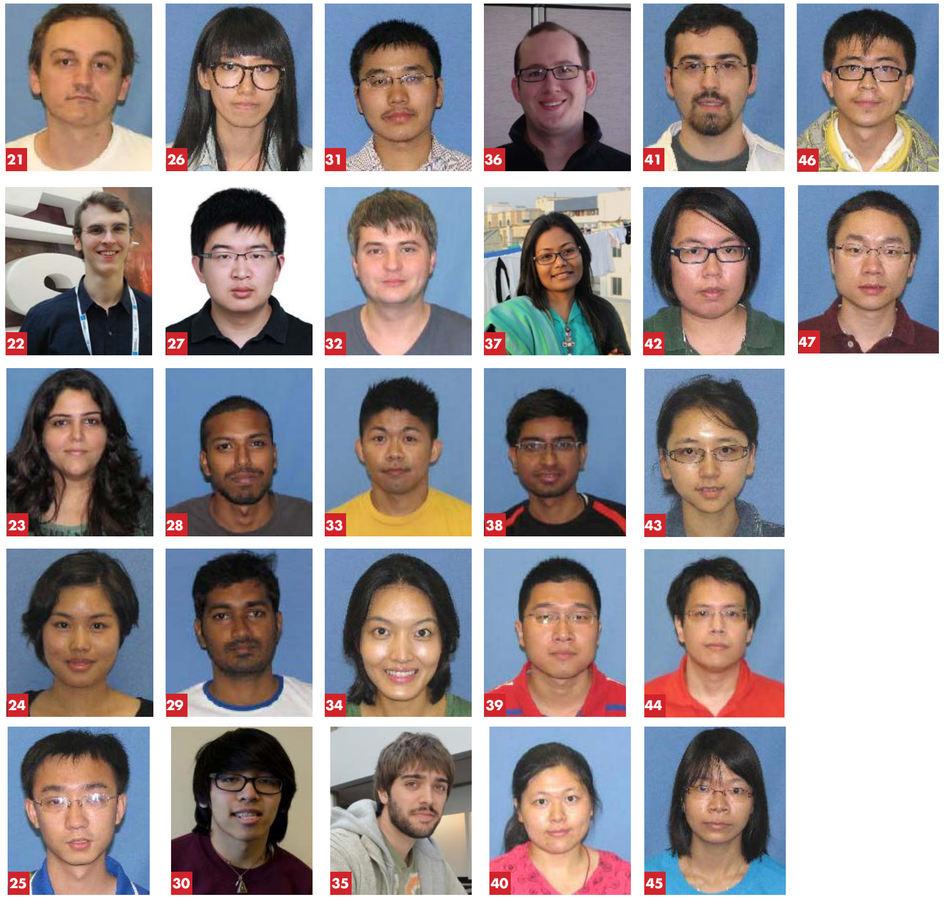
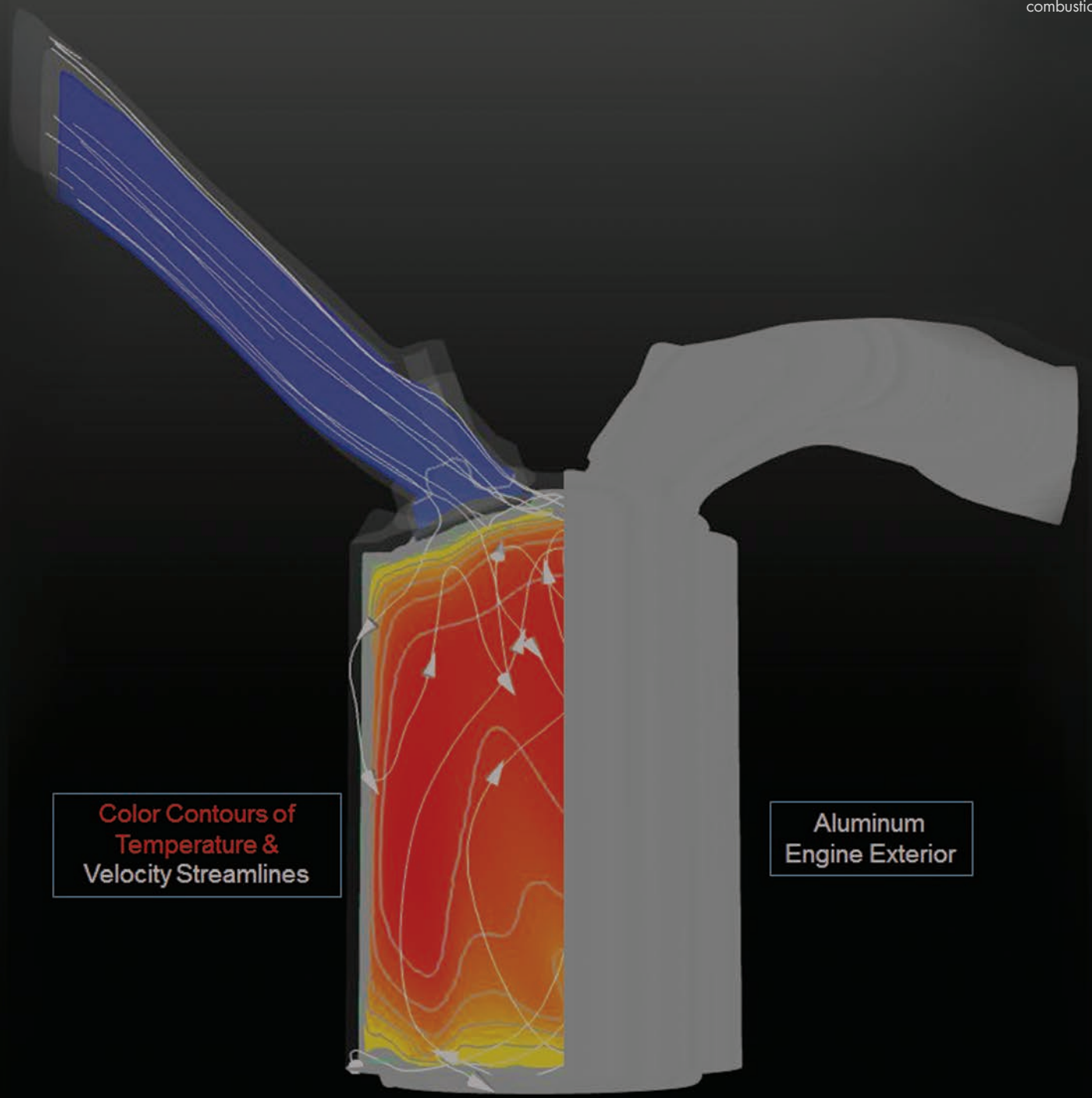


Image by Aimilios Sofianopoulos, Mechanical Engineering
3D Computational Fluid Dynamics (CFD) simulation of spark ignited natural gas combustion in an internal combustion engine



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