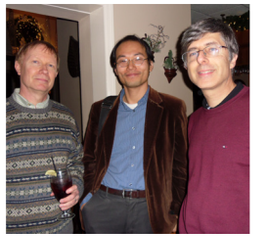
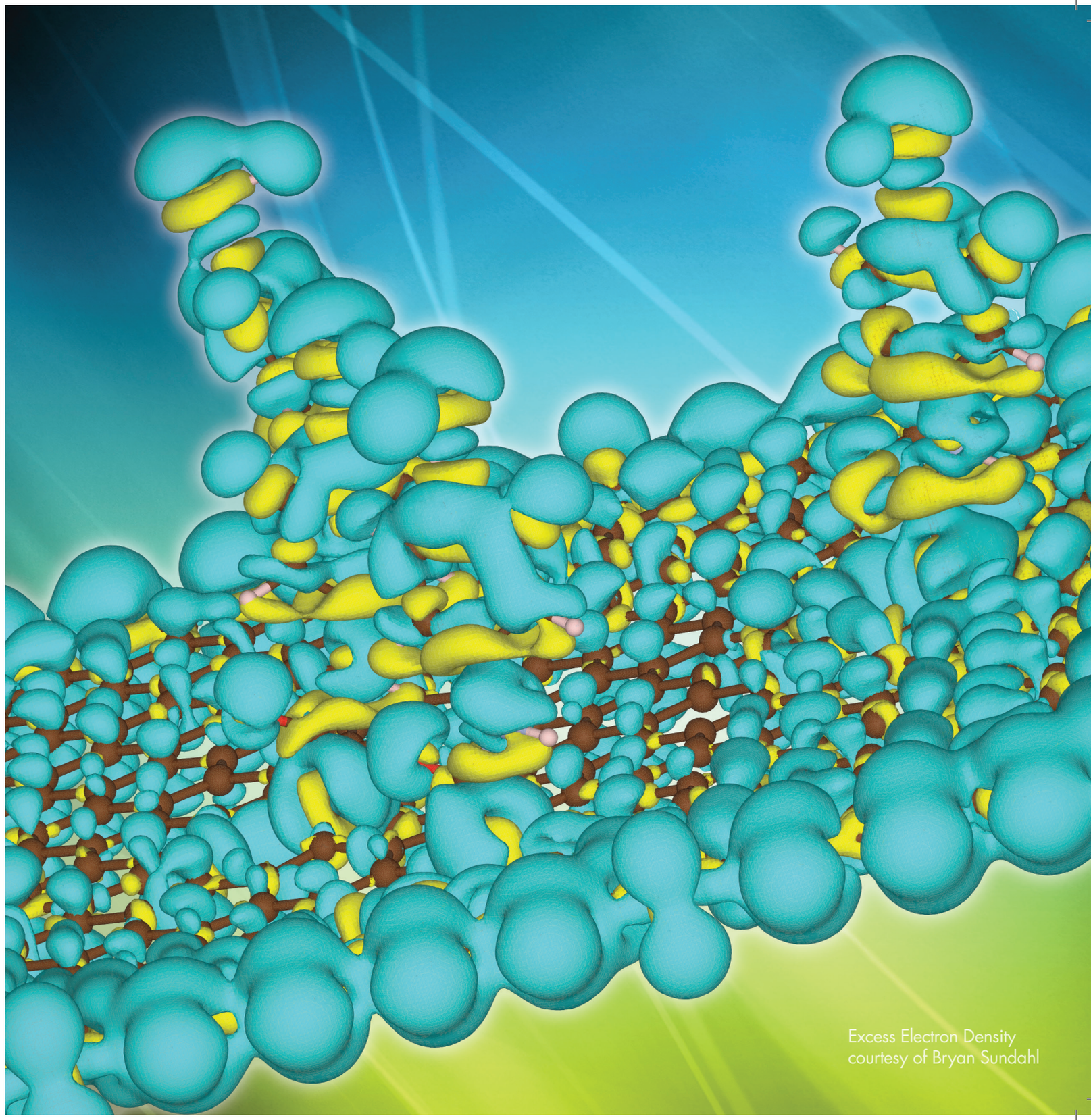
iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

ANNUAL REPORT 2014





Excess Electron Density
courtesy of Bryan Sundahl

MESSAGE FROM THE DIRECTOR

IACS Director Robert Harrison

Dear Friends and Colleagues,

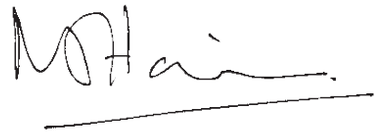
Our second full year has flown by with lots accomplished and many things put in motion, positioning IACS to surge ahead in the coming year. Foremost, it is our excellent faculty and staff that defines us, and this past year we were fortunate to have many people join IACS (pages 4-5). Dr. Matt Reuter is a new core IACS faculty member with an appointment in Applied Mathematics & Statistics (AMS) as an assistant professor. His research in chemical physics is characterized by a rigorous approach to both theory and computation with broad relevance to functional electronic materials (think batteries, molecular-scale electronic devices, electron microscopy, etc.) with strong ties to experiment. Firat Coskun joined us from the medical school as our high-performance computer systems administrator and is already leading the charge in ensuring IACS has world-class cyber infrastructure. Through his dual appointment in DoIT, he is coordinating our activities with research computing across all of SBU. Dr. Jason Trelewicz of Materials Science & Engineering is a new affiliate and serves as the project director for the NYSTAR High-Performance Computing Consortium (HPC^2) activity to which he brings not just great energy and enthusiasm but his experience in industry, startup companies and academia (pages 14-15). In total, we added 15 new affiliate faculty in 2014 for a total of 22, and 45 new students for a total of 105. Welcome everyone!

Our pursuit of external funding continues with 19 proposals submitted from IACS last year for a total of $33,538,224: Of these 5 were awarded for a total of $1,801,422 new funding for SBU. Multiple proposals are still pending, the largest being a National Science Foundation expedition in computer science that proposes research into navigating the post-Moore's law future of computer technology and involves SBU faculty from IACS, AMS, Computer Science (CS) and Sociology. In addition, IACS will be home to the new $1M high-performance cluster with funds from the Long Island Regional Economic Development council. A concerted effort led by IACS has gone into developing a new, SBU-wide graduate Certificate in Data and Computational Science and Engineering (CDCSE) that aims to prepare students for successful research careers that develop, interpret or apply advanced computational and data-centric techniques in their field of study. Still under review by the Graduate School, we hope to start the certificate this fall and aim for a steady-state enrollment of 80 students. The training workshops we regularly hold have become very popular, with registration for a 40-person class now closing in about one hour! This is a clear indicator of the pent-up demand for computational skills and resources on campus (page 6).

IACS owes thanks to many people, especially our generous endowers who resource our vision and the SBU university leadership, specifically President Stanley, Provost Assanis and former Dean Shamash, who have been instrumental in many things including hiring and moving our construction project forward. SBU's new CIO, Cole Camplese, has invested a lot of energy into research computing, and we very much appreciate his support. I must also thank the chairs (Profs. Kaufman and Mitchell) and faculty of the CS and AMS departments who have been supportive of our hiring plans.

Special thanks are due to Dr. Peter Paul who was instrumental in founding IACS - we wish him well in his retirement - and finally to Lynn Allopenna, our hugely effective Administrative Director who is truly the engine behind nearly everything we are today.

Yours sincerely,



MISSION STATEMENT

The mission of the Institute for Advanced Computational Science (IACS) is to make sustained advances in the fundamental techniques of data-centric and high-performance computing and in high-impact applications. Cutting edge, collaborative, and bridging frontiers between disciplines, IACS is a powerful incubator generating ideas that influence SBU, the state, the nation and our international research communities. We are led by inclusive, forward-thinking and world-renowned researchers working in a highly collaborative environment with access to a wide range of resources.

We began with a transformational $10 million anonymous donation plus matching funds of equal value from the Simons Foundation. Our vision is that by 2017 we will be an internationally recognized center growing close to 100 people, including students and staff. We presently have ten core faculty members and 22 affiliate-faculty spanning chemistry, materials by design, condensed matter, astrophysics, atmospheric science, nano-science, sociology, applied mathematics, ecology and evolution, biomedical informatics, mechanical engineering, and computer science. We are actively recruiting two senior endowed positions and two junior positions in computer science and applied mathematics.

We cooperate closely with the Computational Science Center at Brookhaven National Laboratory, and because of this access plus the pervasive entrepreneurial, think-tank culture of support and encouragement at IACS, our students make connections that elevate their careers and electrify their curiosity. Here, a day might begin with a conversation between a chemist and an applied mathematician, and end with plotting a new project with a social scientist and a computational linguist. The common threads are the inherent multidisciplinary nature of modern science, how we compute, and the technology that drives many advances in our fields. Against this backdrop, IACS plays a lead role in connecting science and its people within the academic community and reaching out to help local industries by increasing their ability to adopt the tools of modern simulation and truly effect a change in the world.

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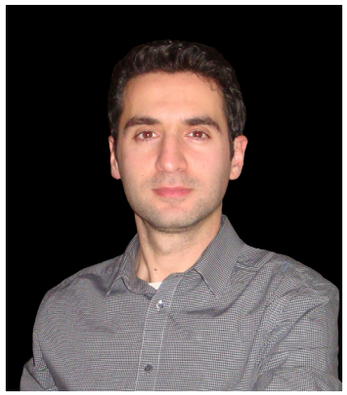
NEW HIRES



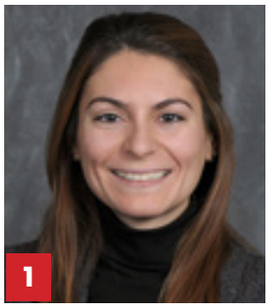
Firat Coskun
Systems Administrator

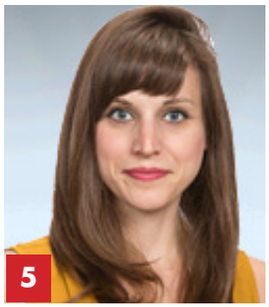
Fırat received his bachelor's degrees in Computer Science and Applied Mathematics & Statistics from Stony Brook University. Prior to starting at the IACS as their Systems Administrator in the fall of 2014, he worked at the Stony Brook School of Medicine for eight years with clinical researchers, and in industry for two years. His interests are in performance-tuning and automation.

Matthew Reuter
Assistant Professor

Before coming to SBU in 2014, Matt Reuter 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 Fellowship for most of his graduate studies at Northwestern.

NEW AFFILIATES





1 Leman Akoglu
Assistant Professor
Computer Science
Stony Brook University

2 Yuefan Deng
Professor
Applied Math & Statistics
Stony Brook University

3 Dilip Gersappe
Professor
Materials Science & Engineering
Stony Brook University

4 James Glimm
Distinguished Professor
Applied Math & Statistics
Stony Brook University

5 Jennifer Heerwig
Assistant Professor
Sociology
Stony Brook University

6 Jason Jones
Assistant Professor
Sociology
Stony Brook University

7 Heather Lynch
Assistant Professor
Ecology & Evolution
Stony Brook University

8 Sotirios Mamalis
Assistant Professor
Mechanical Engineering
Stony Brook University

9 Marek Michalewicz
Senior Director
A*STAR Computational Resource Centre
Singapore

10 Joel Saltz
Professor, Chair
Biomedical Informatics
Stony Brook University

11 Jason Trelewicz
Assistant Professor
Materials Science & Engineering
Stony Brook University

12 Michael White
Professor
Chemistry
Stony Brook University

13 Shinjae Yoo
Associate Computational Scientist
Computational Science Center
Brookhaven National Laboratory

14 Dantong Yu
Group Leader
Computational Science Center
Brookhaven National Laboratory

15 Michael Zingale
Associate Professor
Physics & Astronomy
Stony Brook University

IACS SEMINAR SERIES

February 21, 2014
Steven Gordon The Ohio State University
Preparing the Future Workforce: Careers in Science & Engineering

March 7, 2014
Steve Skiena Stony Brook University
Who's Bigger? A Quantitative Analysis of Historical Fame

March 17, 2014
Michele Parrinello ETH Zurich
Atomistic Simulations: Past, Present and Future

March 19, 2014
Nikos Chrisochoides Old Dominion University
Future Perspectives for Parallel Mesh Generation and Real-Time Image-To-Mesh Conversion for Medical Image Computing

March 24, 2014
Michele Parrinello ETH Zurich
Discussion of Recent Advances in Biochemical Simulations

March 31, 2014
Michele Parrinello ETH Zurich
Discussion of Recent Advances in Simulating Crystal Growth

April 10, 2014
Petr Plechac University of Delaware
Mathematical Strategies for Coarse-graining and Sensitivity Analysis of High-dimensional Stochastic Systems

April 17, 2014
Damon Centola University of Pennsylvania
Social Science Online: The Evolution of Norms

May 5, 2014
Paul Messina Argonne National Laboratory Computational Science at the Argonne Leadership Computing Facility

May 8, 2014
Jennifer Heerwig Stony Brook University
Donations and Dependence: Elite Individual Contributor Strategies in House Elections

May 14, 2014
Eunice Santos University of Texas, El Paso
Effective Modeling and Analysis in Computational Social Systems

May 15, 2014
Jack Wells NCCS Oak Ridge National Laboratory
What Does Titan Tell Us About Preparing for Exascale Supercomputers?

May 20, 2014
Saday Sadayappan The Ohio State University
Domain-specific Abstractions for Compiler Optimization

May 21, 2014
Nikos Chrisochoides Old Dominion University
Towards Exascale Parallel Mesh Generation and Real-Time Medical Image Computing

May 27, 2014
Barbara Chapman University of Houston
Exascale Programming Models: Where Are We Now?

May 29, 2014
Michela Taufer University of Delaware
Enabling Scalable Data Analysis of Large Computational Structural Biology Datasets on Distributed Memory Systems

May 30, 2014
Matthew Reuter Northwestern University
Reconciling Experiment and Theory/Computation in Studies of Electron Transport

June 12, 2014
Terry Haut Los Alamos National Laboratory
Nonlinear Approximations for Electronic Structure Calculations

August 22, 2014
Lucas Lindsay Oak Ridge National Laboratory
First Principles Phonon Thermal Transport

September 11, 2014
Peter Knowles Cardiff University
New Approaches to Predicting and Understanding the Electronic Structure of Molecules

October 2, 2014
Tom Furlani University at Buffalo
Optimizing the Performance of High Performance Computing Systems

October 16, 2014
D.K. Panda The Ohio State University
Designing Software Libraries and Middleware for Exascale Computing: Opportunities and Challenges

October 23, 2014
Carlos Colosqui Stony Brook University
Multiscale Computational Approaches for the Dynamics of Colloidal Systems

October 30, 2014
Javad Mostaghimi University of Toronto
Towards a Complete Model of DC Plasma Spray Process

PROJECTS, PROGRAMS & EVENTS

January 23-24, 2014
Open MP/MPI Workshop
Stony Brook University

March 28-30, 2014
(SICM)2 Parallel Computing Workshop
Stony Brook Manhattan

May 6, 2014
Networking Social
Bliss Restaurant

July 7-18, 2014
Software-Development Summer School for Computational Chemistry and Materials Modeling
Stony Brook University

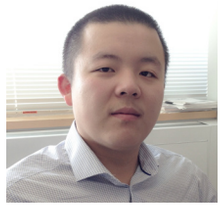
August 21, 2014
OpenMP Workshop Stony Brook University

December 2, 2014
IACS Anniversary Dinner
Fifth Season Restaurant

FROM AMONG HUNDREDS OF APPLICANTS, TWO IACS GRADUATE STUDENTS ARE CHOSEN TO PRESENT AT SUPERCOMPUTING 2014

Two Ph.D. Stony Brook University graduate students in the Applied Mathematics & Statistics Department were chosen to present their research at the Supercomputing 2014 (SC14) annual conference, to be held this year in New Orleans, Louisiana November 17-21.

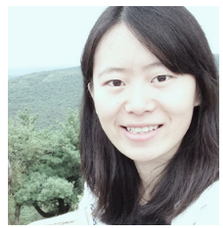
Mr. Li Zhang and Ms. Na Zhang, working with Professor Yuefan Deng who is an affiliate faculty member in the Institute for Advanced Computational Science (IACS), were selected and will present posters at this premier conference where their work will be viewed by a prestigious audience of more than ten thousand from all corners of the world.



"The SC14 Technical Posters program received 193 regular, electronic, and education poster submissions and 44 ACM SRC poster submissions, which covered a wide variety of research topics in HPC," read the acceptance emails sent to the students and their advisor. "The committee has accepted 76 regular, electronic, and education posters and 23 ACM SRC student posters, reflecting an average acceptance of 39% for regular, electronic, and education posters as well as an average acceptance of 52% for the ACM SRC posters."

Li Zhang, an Association for Computing Machinery (ACM) member, was accepted to present at the conference under the ACM Student Research Competition (SRC) category. His poster, "A Molecular Model for Platelets at Multiple Scales and Simulations on Supercomputers," along with a video of his presentation will be available on the conference webpage at http://sc14.supercomputing.org. "I am very excited about being accepted, and it will be my first time to show my work at this wonderful event," said Li. "The ACM SRC is a very competitive program, and I will do my best to present myself, catching up with latest developments of HPC for future study."

Na Zhang will present under the regular and education poster category. Her work is entitled "A Multiple Time Stepping Algorithm for Efficient Multiscale Modeling of Platelets Flowing in Blood Plasma." It will be her second time attending this event: Last year Na presented her work as part of the SC13 Doctoral Showcase Program. "I'm honored to be accepted to present at the prestigious SC14 conference again. I'm very happy to be able to attend this year's SC14 to showcase my latest results and learn more about the impact and new trends of HPC."



Both students' work involves molecular modeling and supercomputing based on platelets biophysics. Their advanced research models platelets at multiple scales with accurate mechanics and dynamics, and successfully simulates these models on high-performance computing resources with updated computational methods. "Their work represents the state-of-the-art applications of supercomputers to problems of vital importance to our health that few other methods can match for quantitative understanding. Like many problems in life sciences and medicine, the study of platelets is very challenging and the students have made baby steps forward. I'm glad the SC14 review committees recognized their efforts," Professor Deng commented proudly.

Association for Computing Machinery (ACM) Student Research Competition Finalists pose for a picture at SuperComputing 2014 held in New Orleans November 16-21. The student from Stony Brook University is IACS Graduate Student Li Zhang who works for Professor Yuefan Deng in the Applied Mathematics & Statistics Department. His poster, "A Molecular Model for Platelets at Multiple Scales and Simulations on Supercomputers," along with a video of his presentation is available to view on the conference webpage at http://sc14.supercomputing.org. The finalists are pictured with Trish Damkroger (LLNL, SC14 General Chair); Jack Dongarra (The University of Tennessee, SC14 Tech Program Chair); Michela Taufer (University of Delaware, SC14 Tech Program co-Chair); and Alice Koniges (LBNL, SC14 Poster deputy Chair).

Li and Na will have their travel supported by the AMS Department for $400 per student. Also, as a participant under the ACM SRC program, Li will be funded up to $500 by the ACM SRC Travel Award, which is sponsored by Microsoft Research. Although both students will be eligible to win best poster awards, if Li wins first place he will be entered into the SRC Grand Finals (Grand Finals are judged over the internet). Winners of the Grand Finals are invited (with their faculty advisor) to the annual ACM Awards Banquet where the ACM Turing Award is presented.

The Institute for Advanced Computational Science engages faculty, students and postdocs from a wide variety of academic backgrounds, all of whom have research interests that involve the use of high-performance and data-intensive computing. The pervasive entrepreneurial, think-tank culture of networking and support at IACS enables those who participate in their events to make connections that elevate careers and electrify curiosity. Students and postdocs conducting research in computational science are of particular interest to institute faculty, and every effort is made to generate support and promote opportunities to help further their careers in relevant fields. To find out more about IACS and the schedule of events, see http://iacs.stonybrook.edu/events.

The Stony Brook team awarded 50 million hours of supercomputing include, from left: Alan Calder, Max Katz, Adam Jacobs and Michael Zingale.

STONY BROOK RESEARCHERS RECEIVE TWO-YEAR INCITE AWARD OF 50 MILLION SUPERCOMPUTING HOURS FOR MODELING ASTROPHYSICAL EXPLOSIONS

A team of Stony Brook University researchers has been awarded 50 million hours on the Titan Cray XK7 at Oak Ridge National Laboratory, one of the world's fastest supercomputers, to advance their research on modeling of astrophysical explosions. The two-year project, titled, "Approaching Exascale Models of Astrophysical Explosions," led by Astronomy Professor Michael Zingale in the Department of Physics and Astronomy, stems from the U.S. Department of Energy's Innovative and Novel Computational Impact on Theory and Experiment award (INCITE), which provides the supercomputing hours.

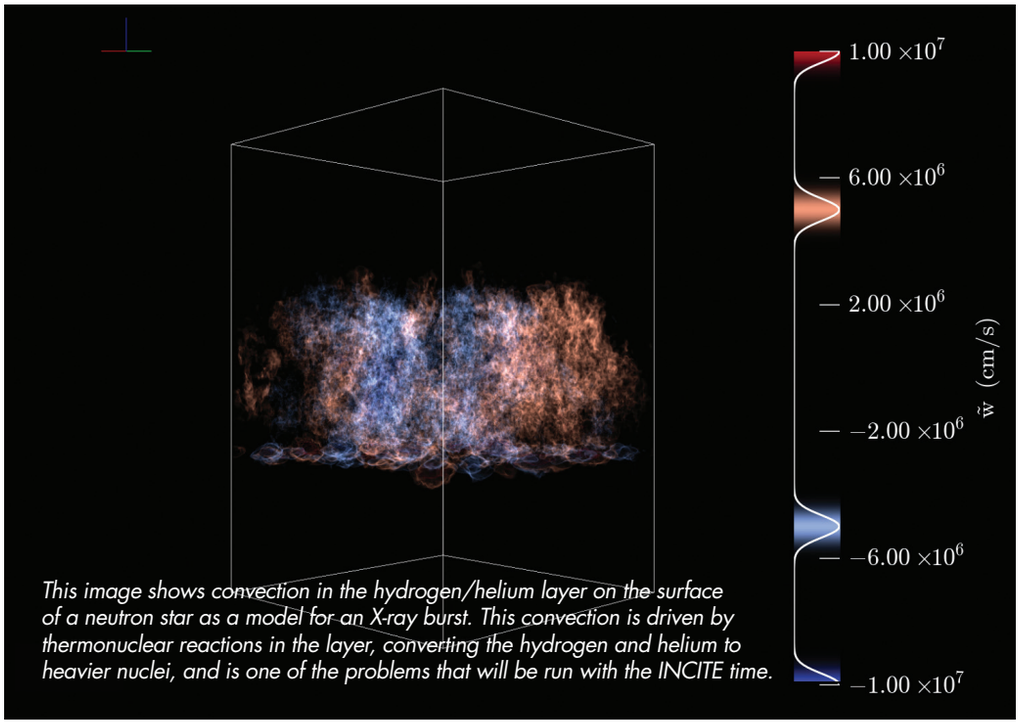
The team is carrying out a comprehensive study of two classes of thermonuclear-powered stellar explosions involving compact objects, type Ia supernovae (SNe Ia) and X-ray bursts (XRBs). Key to their analysis is use of two multiphysics simulation codes, Maestro and Castro, which are specifically designed for the efficient modeling of astrophysical explosions.

"The team's primary goal of the project will be to explore a variety of initial configurations of stellar explosions in the densest stellar objects in the Universe," said Zingale.

Zingale and former SBU graduate student Chris Malone (now at Los Alamos National Laboratory) will explore X-ray bursts, the explosion of surface hydrogen and helium on the surface of a neutron star–a star more massive than our Sun but only 10 kilometers in radius.

The team's award of 50 million computer hours is the equivalent of running calculations on 5,000 processors simultaneously for an entire year. The team will run a variety of simulations during the research, the largest of which will require computing on more than 100,000 processors simultaneously. The computer time will support several graduate student projects, including that of Adam Jacobs, who is exploring ignition in helium shells on the surface of dense stellar remnants and Max Katz, who is modeling the merger of two dense stellar remnants. The time will also support the research of another graduate student, Don Willcox, who recently joined the group. He will be working on the role of convection and the weak nuclear force in progenitor white dwarfs.

"This award will allow us to perform simulations with unprecedented realism to address these fascinating events. It is a great opportunity to advance our understanding of how these things work." said Co-investigator Professor Alan Calder, a member of the Astronomy Group and the Institute for Advanced Computational Science at Stony Brook.



This image shows convection in the hydrogen/helium layer on the surface of a neutron star as a model for an X-ray burst. This convection is driven by thermonuclear reactions in the layer, converting the hydrogen and helium to heavier nuclei, and is one of the problems that will be run with the INCITE time.

"This new INCITE award is a tremendous accomplishment for Profs. Zingale and Calder and their team; it will enable the advancement of knowledge in one of the most cutting-edge areas of astrophysics," said Stony Brook University President Samuel L. Stanley Jr., M.D. "It is remarkable how the U.S. Department of Energy's Office of Science is advancing this field with the important designation of supercomputing time, and Stony Brook University is proud to be able to provide such an opportunity for our faculty and students."

Professor Zingale has received supercomputer hour time from the INCITE program since 2007, and Professor Calder has been part of four different INCITE awards with different collaborations.

Additional Co-Investigators on the project include Ann Almgren and John Bell from Lawrence Berkeley National Laboratory; Chris Malone from Los Alamos National Laboratory; Dan Kasen from University of California Berkeley; and Stan Woosley from University of California Santa Cruz. The entire team has worked on these models and developed simulation codes for about a decade.

The INCITE program promotes transformational advances in science and technology through large allocations of time on state-of-the-art supercomputers the U.S. Department of Energy's leadership computing facilities at Oak Ridge and Argonne National Laboratories. Open to researchers from academia, government labs, and industry, the INCITE program aims to accelerate scientific discoveries and technological innovations that address "grand challenges" in science and engineering.

IACS PEOPLE ON THE MOVE

Robert Harrison

IACS Director Robert Harrison was awarded 15 million processor hours, from the Department of Energy's INCITE Leadership Computing program, on Argonne National Laboratory's IBM Blue Gene/Q for his proposal entitled Dynamic and Adaptive Parallel Programming for Exascale Research. Along with Harrison, the Co-Investigators are George Fann, Oak Ridge National Laboratory; Laura Ratcliff, Argonne National Laboratory; Saday Sadayappan, The Ohio State University; and Edward Valeev, Virginia Tech.

Predrag Krstic

Professors Robert Harrison and Predrag Krstic of IACS were invited speakers at the 2014 Joint ICTP-IAEA conference on Models and Data for Plasma-Material Interaction in Fusion Devices. Krstic presented the talk *The Atomistic Phenomena at the Plasma-surface Interfaces* followed by Harrison's talk *Techniques in Uncertainty Quantification and Initial Application to Plasma-material Interfaces*. The 2014 conference on Models and Data for Plasma-Material Interaction in Fusion Devices was organized by the Abdus Salam International Centre for Theoretical Physics (ICTP, Trieste, Italy) in cooperation with the International Atomic Energy Agency (IAEA, Vienna, Austria).

FERNANDEZ-SERRA'S GROUP USES HANDY TO STUDY ELECTROCHEMISTRY

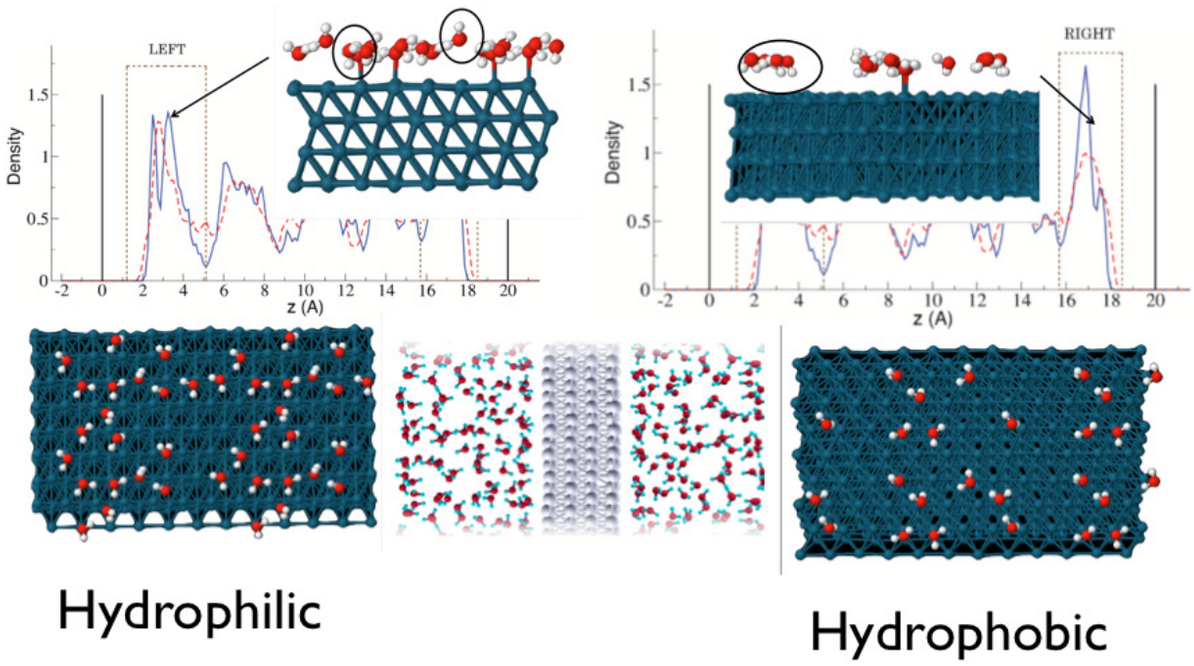


Fig. 1 Distribution of O and H along the z–axis (in Å) for the Pd/H 2O (PBE) simulations

IACS Professor Marivi Fernandez-Serra's group made extensive use this year of the new IACS cluster Handy. In particular, one of the research areas they are most excited about is related to electrochemical energy storage and electrochemistry.

The group is working on the computational modeling of the metal-electrolyte interface purely from first principles. The accurate calculation of the electrostatic potential at electrically biased metal-electrolyte interfaces is a current challenge for periodic "ab-initio" simulations. It is also an essential requisite for predicting the correspondence between the macroscopic voltage and the microscopic interfacial charge distribution in electrochemical fuel cells. This interfacial charge distribution is the result of the chemical bonding between solute and metal atoms, and therefore cannot be accurately calculated with the use of semi-empirical classical force fields.

This year Serra's group worked on producing an accurate method to simulate the water/metal interface. While both experimental and theoretical surface scientists have made a lot of progress on the understanding and characterization of both atomistic structures and reactions at the solid/vacuum interface, the theoretical description of electrochemical interfaces is still lacking. A reason for this is that a complete and accurate first-principles description of both the liquid and the metal interfaces is still computationally too expensive and complex, since their characteristics are governed by the explicit atomic and electronic structure built at the interface as a response to environmental conditions.

In the group's recent paper (Local order of liquid water at metallic electrode surfaces, Luana Pedroza, A. Poisier and M. V. Fernandez-Serra, J. Chem. Phys, 142, 034706 (2015)), they studied the structure and dynamics of liquid water in contact with Pd and Au (111) surfaces using ab initio molecular dynamics simulations with and without van der Waals interactions. Results show that the structure of water at the interface of these two metals is very different. For Pd, they observed the formation of two different domains of preferred orientations, with opposite net interfacial dipoles. One of these two domains had a large degree of in-plane hexagonal order. For Au, a single domain existed with no in-plane order. For both metals, the structure of liquid water at the interface was strongly dependent on the use of dispersion forces. The origin of the structural domains observed in Pd is associated with the interplay between water/water and water/metal interactions. This effect is strongly dependent on the charge transfer that occurs at the interface and which is not modeled by current state-of-the-art semi-empirical force fields.

KRSTIC STUDIES PHYSICAL MODELS FOR RECOGNITION TUNNELING

Professor Predrag Krstic of IACS, Stony Brook University, used the Handy Cluster for a set of calculations that led to the development of the physical model for recognition tunneling (Nanotechnology IOP 26, (2015) 084001)

Recognition tunneling (RT) is the experimental method developed and used for third-generation DNA sequencing as well as for detection and recognition of amino acids, peptides, and sugars by the Biodesign Institute of the Arizona State University. This method provides a new type of single molecule sensor which directly probes the chemical bonds at a molecular level, which has significantly increased discrimination of the electron tunneling signals obtained from each of the DNA bases and is now becoming a good candidate as a "reading head" for DNA sequencing. Using an electron-tunneling signal, it identifies target molecules trapped between tunneling electrodes functionalized with recognition molecules (imidazole-carboxamide readers, referred to here as ICA) that serve as specific chemical linkages between the metal electrodes and the trapped target molecule, like any one of the four DNA bases. ICA forms non-covalent contacts with the target molecules that are strongly bonded to the metal electrodes (Fig. 1a). The weak non-covalent bonding of the readers with DNA nucleotides allows for DNA translocation through a pore but slows down the translocation of the DNA segment through the configuring nanopore by some three orders of magnitude. These non-covalent bonds are strong enough to increase signal-to-noise ratio by imposing constraints on thermal fluctuations, elevated by the water environment (Fig. 1b).

Through our simulations we answered several big questions about RT: (1) Is the magnitude of the observed signals compatible with electron tunneling? (2) Does a reasonable physical model of the fluctuations predict the form of the RT signal? (3) Do the RT signals in a model system change enough with the chemistry of the target molecule (in the simulation) to allow a machine learning algorithm to identify individual signal spikes with significant accuracy?

To extend the time scale toward ms, we adapted a simplified, coarse-grain model of DNA (the oxDNA Model developed at the University of Oxford (UK)) to extend classical dynamics simulations into the much longer time scales (covering ns-μs-ms ranges). We extracted the hydrogen bond stretching and developed a simplified representation of ICA molecules interacting with all DNA bases. Using the calculated values of the hydrogen bond stretching over large time spans in the tunneling decay model, we calculated the time dependence of the corresponding RT signals (Fig. 2).

The calculated signals bear a strong resemblance to measured RT signals. Finally, we took calculated RT signals for all four bases interacting with the model ICA molecule and analyzed them with the SVM. Each signal spike could be correctly assigned (A, T, G or C) to an accuracy that approached 80% for bases where adequate training data were available. This provided a theoretical underpinning for the experimental observation that individual signal spikes could be assigned to better than 90% accuracy if adequate training data were available.

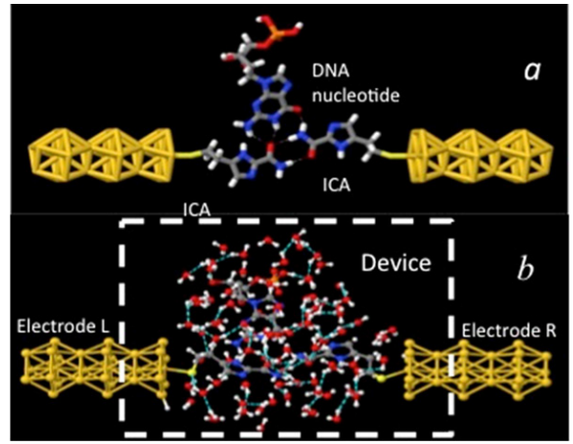


Fig. 1. (a) Recognition molecules (ICA) covalently bound to gold electrodes, form transient hydrogen bonds (dashed lines) with a DNA base (guanosine in this example) to bridge the gap between the electrodes. This complex serves as the model system for the NEGF simulation of the recognition tunneling current signals performed on the IACS Handy Cluster. (b) A much more complex pattern of hydrogen bonds emerges when the complex is embedded in a bath of 90 water molecules. Color key: red-oxygen, white-hydrogen, blue-nitrogen, gray-carbon, yellow-gold atoms.

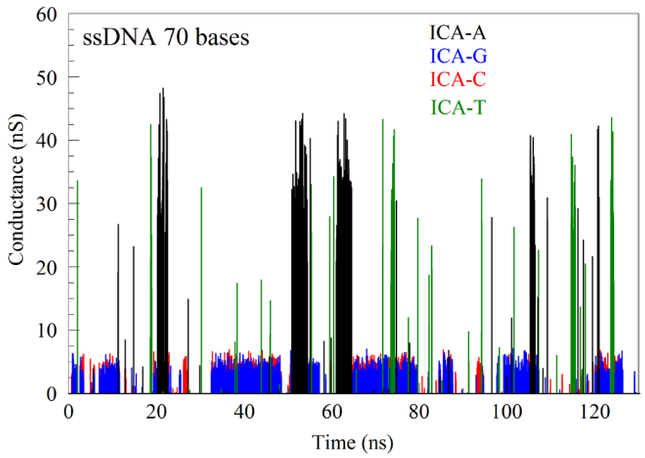


Fig. 2. Calculated hydrogen-bond conductance between ICA-probes and various bases in a 70-tuple heterogeneous DNA which contains all 4 bases (GCCGTTCGCACGGCGCG AAGGAGCGGCTGCCAGTTCCAAGTGCGGACGCGG CTGCCGCAACGGAGCTCGT.) The RT Signal form G and C are much smaller because of the current scaling choice. The frequency of the peaks for various bond-types is also a visible characteristic.

IACS ASSOCIATE DILIP GERSAPPE USES HANDY TO STUDY

Rheology of Poly (N-isopropylacrylamide)-Clay Nanocomposite Hydrogels

By Di Xu and Dilip Gersappe

Polyacrylamide (PA) has long been known for its ability to swell in water to make soft clear gels. Since the discovery that poly(N-isopropylacrylamide) (PNIPA), a variant of PA, exhibits a lower critical solution temperature attributed to a coil to globule transition, study of this material intensified. Unfortunately it was found to exhibit relatively brittle behavior compared to its PA predecessor, thus limiting its use for biological and industrial applications. The discovery of using clay to tune the properties of PNIPA showed that it was possible to make a strong nanocomposite (NC) hydrogel that was thermally responsive within a physiological temperature range. This enabled numerous applications for PNIPA, such as: drug delivery systems rapid release cell culture substrates flocculation additives,1 separation devices and wound healing dressings.

Earlier studies of polymer-clay gels focused on regimes above the gelation point (or didn't explicitly distinguish gelation threshold). Further, the subtle mechanical changes and structure at the gelation point have not been studied. Such studies would yield valuable information into the formation of these networks and the factors that control their formation. Our goal in this work was to use theoretical studies to examine the onset of gelation in PNIPA-clay gels and the mechanisms that control the properties of these gels. We used Molecular Dynamics (MD) simulations to study the rheology of polymer-clay nanocomposite hydrogels. The MD simulations studied the formation of physical networks as a function of the clay concentration. Simulations showed that while the local structure changed from isolated polymer-clay clusters to a percolating network with increasing clay concentration, the networks were only able to sustain stress at concentrations of roughly 1.5 times the percolation transition. Our results showed excellent agreement with experimental studies.

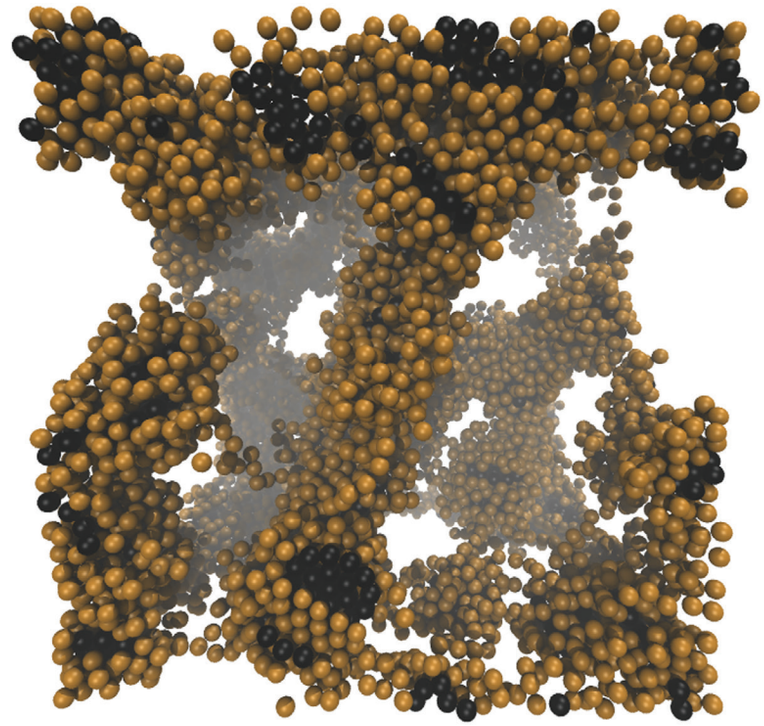


Fig. 1. Image from the simulation showing the structure of the hydrogel. The clay particles are in black and the polymer chains are in brown. Solvent molecules are not shown for clarity.

TWO RESEARCH TOPICS IN MATERIALS SCIENCE

Modeling Tablet Dissolution in Complex Hydrodynamic Environments

By Ning Sun and Dilip Gersappe

As a regulatory requirement mandated by the FDA, the dissolution test is critical in the drug development process. Even though a standardized apparatus for the dissolution test has been set up for over 30 years, the hydrodynamics within the dissolution apparatus have not been fully understood, and large variations in dissolution tests have been reported. While failed dissolution tests can result in costly product recalls, as long as we don't have a mechanistic understanding of the process, reasons for failure will be difficult to resolve. Computational methods can enable us to study this system at a level of detail not always accessible by experiments, in order to develop a fundamental understanding of the interplay between the complex processes that control dissolution. Our goal was to develop a predictive computational method that uses experimental data to determine the dissolution mechanism of drugs in a complex hydrodynamic environment.

In this work we used the Lattice Boltzmann Model to solve the dissolution process and the flow field together by defining the boundary conditions of the dissolution process according to the local concentration gradient that is in turn influenced by the local velocity. We also included the disintegration term in the dissolution by setting up critical local velocities, and implemented the body force according to the movement of stirring paddle. A dynamic boundary dependent on the dissolution process was incorporated into the system so that the geometric changes of tablet morphology were also considered. Through this approach, a real flow field in the USP Apparatus II could be recovered and the influence of the flow field on the dissolution process could be studied.

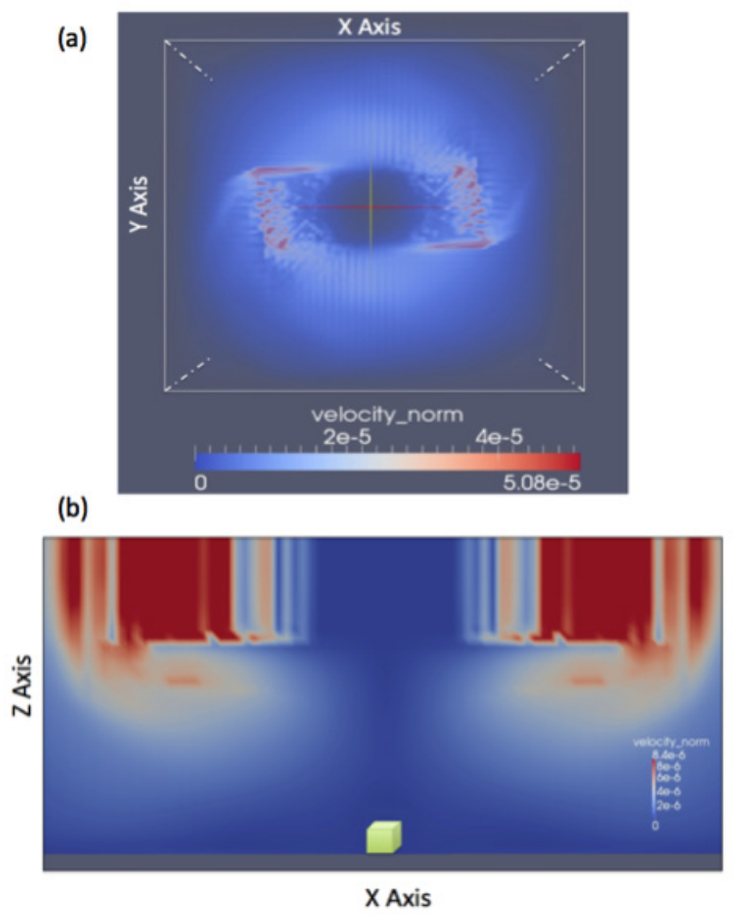


Fig. 2. (top) Velocity magnitude in the whole system viewed from the x-y plane at a paddle speed of 50 rpm. (bottom) Velocity magnitude in the region above the tablet (green in the figure) in the X-Z plane at paddle speed of 50 rpm.

hpc² | Improved Simulation Through Collaboration

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NEW YORK STATE HIGH PERFORMANCE COMPUTATION CONSORTIUM (HPC²)

The New York State High Performance Computation Consortium (HPC²) is a three-year NYSTAR funded program that brings together computing expertise from the IACS at Stony Brook University, Brookhaven National Laboratory, Rensselaer Polytechnic Institute, the Center for Computational Research at SUNY Buffalo, the Mount Sinai School of Medicine, and Marist College. The mission of the consortium is to engage New York State companies on the use of advanced computing and data analytics for improving productivity, developing new products, and fostering innovation to provide them with a competitive advantage in growing their businesses. A core HPC² team has been established at Stony Brook University including the PI Dr. Robert Harrison, the Program Director Dr. Jason Trelewicz, and five additional faculty members in the College of Engineering and Applied Sciences. The high-performance computational resources and data capabilities of IACS and Brookhaven National Laboratory are being leveraged by the team to address problem-solving and design needs communicated by their industrial partners. The projects summarized here were selected to provide a diversified computing portfolio for the HPC² program that incorporate a range of coding and simulation techniques including code translation technologies, molecular dynamics simulations, computational fluid dynamics, and solid modeling.

SOURCE-TO-SOURCE TRANSLATOR FOR HIGH-PERFORMANCE COMPUTING WITH R LANGUAGE

Project Lead: Xiangmin Jiao, Department of Applied Mathematics and Statistics

Industrial Partner: ParaLab Computing, LLC

The team at Stony Brook University, led by Professor Xiangmin Jiao in the Department of Applied Mathematics and Statistics, is working with ParaLab Computing, LLC on the development of a new source-to-source technology to translate user-written R codes into high-performance C++ codes with a myriad of commercial applications in the insurance, advertising, and pharmaceutical industries.

ENABLING STABLE NANOCRYSTALLINE TUNGSTEN ALLOYS AS PLASMA FACING MATERIALS FOR FUSION REACTORS

Project Lead: Jason Trelewicz, Department of Materials Science and Engineering

Industrial Partner: TheoretiK

Plasma-facing components for reactor scale fusion devices require materials to operate under far-from-equilibrium conditions of extreme temperature, radiation, and stress. The team in the Department of Materials Science and Engineering, under the direction of Professor Jason Trelewicz, is employing predictive thermodynamic modeling and atomistic simulations to study nanograin stability, radiation tolerance, and mechanical behavior of nanostructured tungsten alloys.

PARTIAL REFORMATION OF MIXED FUELS FOR COMBUSTION IN HEAVY-DUTY ENGINES – A MODELING STUDY

Project Lead: Sotirios Mamalis, Department of Mechanical Engineering

Industrial Partner: Innoveering, LLC

Heavy-duty diesel engines are often operated using fuels of mixed properties (thermodynamic and chemical) that have variable hydrocarbon as well as CO^2 content, resulting in inefficient combustion and non-robust engine operation. To address these and other issues, the team in the Department of Mechanical Engineering led by Professor Sotirios Mamalis and partnered with Innoveering, LLC is studying how to enable decomposition (a.k.a., reformation) of larger hydrocarbon molecules into smaller, more reactive species. Computational fluid dynamics simulations are being employed to perform chemistry and heat transfer calculations to assess combustion efficiency and predict emission formations with direct application to diesel engines.

MOLECULAR DYNAMICS STUDY OF SULFUR CRYSTALS FOR SUSTAINABLE CONCRETE

Project Lead: Juhyuk Moon, Department of Civil Engineering

Industrial Partner: Green SulfCrete, LLC

Concrete is the most widely used manufacturing material, with global concrete production exceeding 20 billion tons each year, but the energy consumed results in 5~7% of global CO^2 emissions. The team in the Civil Engineering Department, led by Professor Juhyuk Moon, is working with Green SulfCrete, LLC on the development and commercialization of new green concrete based on sulfur, denoted "SulfCrete," which is produced by the recycling of industrial by-product materials of sulfur, fly ash, and catalytic cracking oil. Molecular dynamics simulations are being used to understand the different thermal behavior of sulfur polymorphs using the large-scale atomic/molecular massively parallel simulator (LAMMPS) platform.

COMPUTATIONAL MODELING OF THE THERMOMECHANICAL PROPERTIES OF THE REGENERATOR IN A THERMALLY DRIVEN HEAT PUMP

Project Lead: T. A. Venkatesh, Department of Materials Science and Engineering, and Maen Alkhader, Department of Mechanical Engineering

Industrial Partner: ThermoLift, Inc.

ThermoLift is developing a disruptive and transformational thermally-driven heat pump that provides heating, cooling, and hot water all in one device. Materials selection issues for various components such as the hot end, cold end, heat exchangers, and regenerators play a crucial role in determining the efficiency of the heat pump. The team at Stony Brook University, including Professors T.A. Venkatesh and Maen Alkhader, are developing finite element based computational models for controlling thermal and mechanical coupling and predicting thermal history.

PEROZZI AND JACOBS WIN IACS JUNIOR RESEARCHER FELLOWSHIPS

Award includes $32K stipend, $4K for travel

Bryan Perozzi

Adam Jacobs

While studying mathematical models of related objects may not seem relevant to most people, this area of research has many everyday, applications: filling in missing data for social network users and electronic healthcare records; detecting online fraud; discovering attributes of proteins from their interactions; and the list goes on. Graph mining, as it is called, is the subject studied by IACS student Bryan Perozzi, one of this year's winners of the Institute for Advanced Computational Science (IACS) 2014 Junior Researcher Fellowship.

"I'm honored to receive the Junior Researcher Fellowship from IACS," said Perozzi. "Its support opens new options for presenting my work, allowing me to broaden my participation in the global discussion on mining and modeling large attributed graphs."

This is the first year IACS has offered this fellowship, which is for advanced PhD students who are studying computational science with a core member of the institute. "All of the applicants were involved in exciting research, and it is wonderful to see such talent in the IACS community," said IACS Director Robert Harrison. "It was certainly tough choosing two from the excellent pool of candidates, but Perozzi and Jacobs stood out from the crowd because of the passion with which they spoke about their research; the sophistication, breadth and depth of the computational science tools they are employing; and the significance of the potential outcomes of their accomplishments."

The award comes with an increase to the students' stipends to $32,000 plus $4,000 for travel. There were 16 applicants, five of whom were chosen to give 20-minute presentations to the fellowship committee. Out of the five who presented, the two winners were Perozzi, from the Computer Science Department studying under Professor Steven Skiena, and Adam Jacobs, from the Physics & Astronomy Department studying under Associate Professor Michael Zingale.

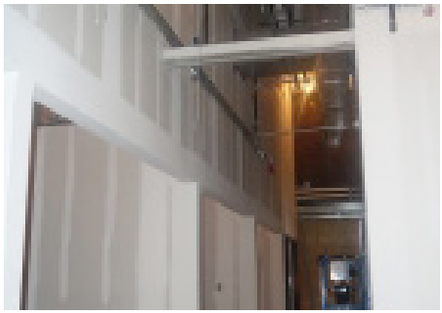
Jacobs studies Type Ia Supernova explosions, which are among the most violent explosions in the universe and therefore bright enough that you can see them from far away. Explosions don't happen that often in any one galaxy, but there are enough galaxies that you can see these Type Ia Supernova explosions regularly, and studying these explosions allows scientist to accurately measure distances in the universe. The main science application for Jacobs' research is to enable cosmologists to more precisely study the physical universe: how it has evolved; what it is composed of; what will be the fate of the universe in the future. On a more applied note, the computational tools Jacobs develops for astrophysical studies can be used by collaborators at Lawrence Berkeley National Laboratory (LBL) investigating combustion. LBL's combustion research provides insight to engineers tackling problems such as reducing pollution and increasing fuel efficiency.

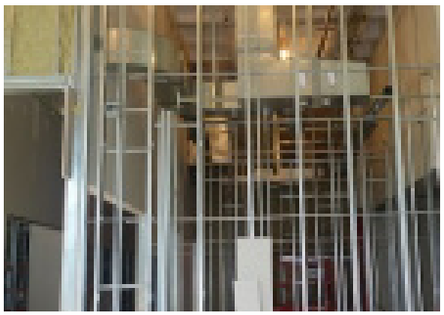
Upon learning that he was one of the fellowship winners, Jacobs said, "I was thrilled when I heard about the award! Over the next year I will be searching for postdoc positions. The award will both make me more competitive and make it possible to travel to computational conferences that the grant I'm funded by now doesn't cover. The award enables a level of research and interdisciplinary exploration that would be otherwise impossible."

> "I WAS THRILLED WHEN I HEARD ABOUT THE AWARD!…THE AWARD ENABLES A LEVEL OF RESEARCH AND INTERDISCIPLINARY EXPLORATION THAT WOULD BE OTHERWISE IMPOSSIBLE."

These fellowships 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 of whom have research interests that involve the use of high-performance and data-intensive computing. To find out more about IACS and the schedule of events, see http://iacs.stonybrook.edu/.

NEW DIGS READY THIS SPRING





Plans are in place for IACS to move into our newly renovated space at the end of April, 2015. Our new location is in the Old Life Sciences Library neighboring the Laufer Center. Features of this new space include a 45-seat multi-purpose room; 18 offices; a full-service kitchen; two conference rooms; and a 35-seat open area for graduate students. In the multi-purpose space, the conference rooms and in the Director's office there will be state-of-the-art AV systems including multifunctional overhead and LCD screens with both professional and desktop video conferencing capabilities supported.

A 10-gigabit network backbone will be used to connect the faculty and staff's workstations to each other, to the High-Performance Cluster (HPC) and out to the rest of the academic research world. Ten times faster than the current generation of gigabit networks, this high bandwidth network infrastructure will be capable of transferring a full DVD in 4 seconds and an entire Blu-ray disc within 20 seconds.

The datacenter for the IACS, located in the mezzanine of the building, will be housing the HPC and similar computational research resources. This space, which is being constructed in phases, will be capable of housing 200 compute nodes by the completion of the first phase. At full capacity the datacenter is projected to be capable of housing 700 nodes with an estimated compute power in the PetaFlop range. In terms of conventional computers, this would roughly be the equivalent of 20,000+ laptops. The intent of the overall space is to cultivate the exchange of ideas across disciplines and to encourage forward thinking in a highly collaborative environment where members and visitors will have access to a wide range of resources.

FUTURE PLANS

Here's a taste of what 2015 will hold for IACS:

1. We will move into our space in May -- Co-location of our faculty and students will transform the dynamics of IACS and greatly enhance cross-disciplinary interactions.

2. New faculty hires -- We anticipate multiple exciting announcements and will continue our search for endowed chairs as well as junior and senior faculty.

3. Joint actions with BNL -- The successful re-competition of the Brookhaven Science Associates' contract to operate Brookhaven National Laboratory (BNL) leads to a greatly expanded commitment to scientific computing at BNL, including up to 20 joint hires with SBU.

4. IACS Computes! -- This summer we will hold our first annual 5-day camp to introduce high-school students to the programming skills and technologies that drive advances in science, industry, business and society.

5. NYSDS -- Co-organized with BNL, the New York Scientific Data Summit (August 2-5) is our first annual national meeting in data-driven discovery.

6. LI-IDEAS -- The proposed Long Island Institute for Data-Enabled Applications is a case of thinking big! Watch this space.

7. LIRED cluster -- This $1M computer will be operational in the summer and brings resources in HPC and big data to SBU, BNL and local industry. It effectively quadruples the size of our present cluster Handy.

8. Expanded training -- Dr. Thornton will lead our charge to hold multiple training workshops on various computational science topics throughout the year.

9. CDCSE -- We hope our advanced graduate Certificate in Data and Computational Science and Engineering will be available this fall.

IACS STUDENT DREAMS BIG FOR HERSELF AND FOR THE FUTURE OF ALL WOMEN

Ph.D. candidate Jesmin Jahan Tithi attends SC14 Women in HPC workshop

By Erica Cirino

Jesmin Jahan Tithi, a fourth-year computer science PhD candidate at Stony Brook University, said that receiving the honor to both attend and present at a prominent international supercomputing conference was "a great opportunity. There were around 10,000 attendees from researchers to students, professors, government organizations, labs and industry from all over the world."

The SuperComputing Conference is an annual event, this year dubbed "SC14" and held from November 16 to 21, 2014 at the Ernest N. Morial Convention Center in New Orleans, Louisiana. The theme of this year's conference was HPC matters (High-Performance Computing), and a major highlight of the conference, said Tithi, was participating in its first-ever "Women in HPC: Mentorship and Leadership" workshop, which featured only two student presentations, one of which was Tithi's. This particular type of women-centric computer science workshop and others like it, she said, have important implications for the future. "In general, more women need to be brought into the STEM fields [science, technology, engineering and math]," said Tithi. She added that a major goal of the workshop is to help more women, particularly women from developing countries, pursue educational and professional futures in computer science.

Men currently dominate the computer science field with the number of women having decreased over time since the early 1980s, according to an October 2014 NPR report titled "When Women Stopped Coding." The report cites one possible reason being that when computers were first made available to the general public, the advertisements were targeted to boys. In addition, an AAUW analysis of 2011 US Census Bureau data shows gender gaps in pay, with women in all STEM fields being paid significantly less than men. These elements combined can work to discourage women from pursuing a future in STEM.

But Tithi says that she is hopeful that workshops like the one she attended at SC14 can help give women the information, support and confidence they need to ultimately be successful in whichever STEM areas they choose. "By meeting together," said Tithi, "women are able to discuss their research, ideas and also any problems they are facing in their field today, and this is very helpful."

left to right: Li Zhang, Jesmin Tithi, Na Zhang attend SC14

Tithi's enthusiasm for bringing women into the STEM fields did not go unnoticed by SC14 organizers. In fact, Tithi said that she was personally invited to write a proposal for the women-centric HPC workshop at next year's conference. Though the four-hour workshop for women at SC14 was excellent, said Tithi, there is room for improvement at next year's event. "I think the next workshop should be bigger and more of an all-day affair," said Tithi. "That way, more women could attend, and there would be enough time to present more research and hold more professional training and networking sessions."

Another high point of the conference for Tithi was presenting her own research during the women-centric workshop, on a paper she recently co-authored on how to boost the energy efficiency of computer processors titled, "Exploiting Spatial Architectures for Edit Distance Algorithms." Tithi said that she was excited to receive "great" feedback on her presentation from the crowd of academics, professionals and industry leaders who attended the conference.

Though attending seminars, talks and workshops at the conference all day during her stay in Louisiana was a little exhausting, Tithi said that on the last day of her trip she finally found a little downtime. "Though I only got to explore the city of New Orleans for a few hours, I am glad I did." Overall, she said, attending SC14 was a rewarding experience, and she is looking forward to next year's conference.

Tithi would like to thank the IACS for funding her trip to SC14. She would also like to thank her advisor, Dr. Rezaul A. Chowdhury, assistant professor of computer science at Stony Brook University, who encouraged her to apply for a spot at the conference. To access the abstract for Tithi's talk, you can visit http://www.womeninhpc.org.uk/sc14/sc14-workshop-speakers-and-contributors#Tithi.

By Alyssa Melillo

Earlier in 2014, Tithi won a prestigious scholarship from the Association for Computing Machinery – Women (ACM-W), an organization dedicated to supporting, celebrating, and advocating for women in all aspects of computing. The maximum number of awards made worldwide by ACM is 36, and each applicant is eligible to receive the award only once. She used the $600 award to help defray the cost of travel to the 2014 International Parallel and Distributed Processing Symposium that was held May 19-23 at the Arizona Grand Resort in Phoenix. At the symposium, Tithi presented a poster on high-performance computing and algorithms, her specific area of study, and participated in a Ph.D. forum. Ultimately Tithi would like to work for either Google or Microsoft on developing and building new computing products.

AWARDS

Jr. Researcher Fellowship
Bryan Perozzi, Computer Science
Skiena

Jr. Researcher Fellowship
Adam Jacobs, Physics & Astronomy
Zingale, Calder

Travel Award
Seetha Pothapragada, AMS
Deng

Travel Award
Li Zhang, AMS
Deng

Travel Award
Jesmin Jahan Tithi, Computer Science
Chowdhury

Writing Award
Pramod Ganapathi, Computer Science
Chowdhury

Writing Award
Dan Elton, Physics & Astronomy
Fernandez-Serra

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1 Alan C. Calder Associate Professor

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 University and then came to Stony Brook'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 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.

7 Predrag Krstic Research Professor

Dr. Predrag Krstic is a Research Professor at the Institute for Advanced Computational Science, a senior staff scientist at the Joint Institute for Computational Sciences, an adjunct professor in the Department of Physics and Astronomy at the University of Tennessee, and founder and owner of the TheoretiK consulting. He has worked in the Physics Division at Oak Ridge National Laboratory in the Theoretical Atomic Physics program since 1995, where he retired as a member of the senior research and development staff and project manager. He obtained his Ph.D. at CC of CUNY in 1981 on the theory of multiphoton processes, and he received his BSC and MSC in technical physics and technical plasma physics from the University of Belgrade. 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 bionanotechnology. His work has been disseminated in more than 200 papers in peer-reviewed journals, in several patents, in more than 80 talks at scientific conferences and seminars, and in a number of international atomic databases. He is a contributor to book chapters; an editor of a number of conference proceedings; a PI and Co-PI on many grants with DOE, NIH, NSF, and IAEA; a consultant for the International Atomic Energy Agency; a Fellow of the American Physical Society; and an organizer and co-organizer for various international conferences.

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 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.

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. In 2014 we have:

- *Supported travel for 21 visitors to the institute;*
- *Featured 31 speakers from around the world in our IACS Seminar Series;*
- *Held one 2-day and one 1-day graduate student workshop (40 SBU registrants each), one 2-week graduate student conference (35 participants nationwide) and one 2-day faculty workshop (22 participants nationwide);*
- *Held 2 social events: Graduate Student Networking Social (35 SBU attendees) and IACS Annual Anniversary Dinner (40 SBU attendees);*
- *Awarded 2 Junior Researcher Fellowships, 2 Young Writers Awards; and 3 Travel Awards;*
- *Hired a Systems Administrator and an Assistant Professor;*
- *Submitted 18 grants; and*
- *Collaborated, trained and supported 3 graduate interns.*

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

- *Recruiting four more faculty plus two endowed chairs;*
- *Moving into our new state-of-the-art offices;*
- *Developing more funding opportunities including those that benefit from focused NYS and on-campus matching funds;*
- *Purchasing another high-performance computing system; and*
- *Building a world-class, pervasive computational infrastructure and technical support to free faculty and students to focus on creativity and innovation.*

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March	Nikos Chrisochoides	Professor	Old Dominion University
March	Michele Parrinello	Professor	ETH Zurich
April	David Keyes	Professor	King Abdullah University of Science and Technology
April	Damon Centola	Associate Professor	University of Pennsylvania
April	Petr Plechac	Professor	University of Delaware
May	Paul Messina	Director of Science	Argonne National Laboratory
May	Saday Sadayappan	Professor	The Ohio State University
May	Eunice Santos	Professor	University of Texas, El Paso
May	Michela Taufer	Associate Professor	University of Delaware
May	Jack Wells	Director of Science	NCCS Oak Ridge National Laboratory
May	Barbara Chapman	Professor	University of Houston
May	Matthew Reuter	Research Associate	Northwestern University
June	Terry Haut	Doctor	Los Alamos National Laboratory
August	Steve Binkley	Director	ACSR Department of Energy
August	Lucas Lindsay	Doctor	Oak Ridge National Laboratory
September	Peter Knowles	Professor	Cardiff University
September	Hideo Sekino	Professor	Tokyo Institute of Technology
October	Tom Furlani	Professor	University at Buffalo
October	Javad Mostaghimi	Professor	University of Toronto
October	D.K. Panda	Professor	The Ohio State University

STUDENTS

1 Sonal Aggarwal
2 Afife Idil Akin
3 Diego Alfaro
4 Aniket Alshi
5 Tianshu Bao
6 Xue Cai
7 Rebecca Conley
8 Sheridan Curley
9 Mahdi Davari
10 Tristan Delaney
11 Simon Divilov
12 Huafeng Dong
13 Daniel Elton
14 Lonia Friedlander
15 Pramod Ganapathi
16 Sohil Gandhi
17 Aditi Ghai
18 Mohammad Mahdi Javanmard
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20 Gautam Kumar
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22 Bingxi Li
23 Hongxu Liu
24 Yue Liu
25 Cao Lu
26 Vivek Pradhan
27 Guangrui Qian
28 Maksim Rakitin
29 Hyang-Gi Song
30 Adrian Soto
31 Bryan Sundahl
32 Jesmin Jahan Tithi
33 Xuebin Wang
34 Shengnan Wang
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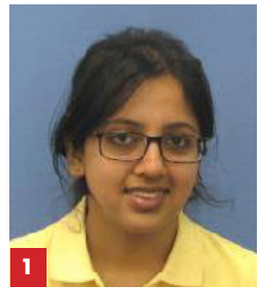
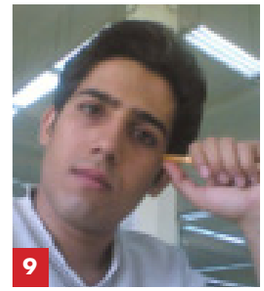
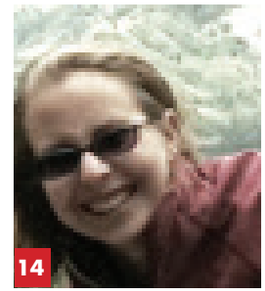
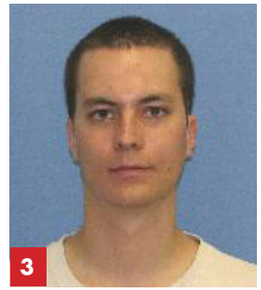
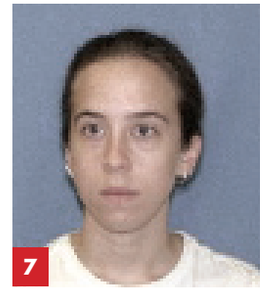
36 Yunpeng Xiao
37 Hongfei Xu
38 Junyi Yang
39 Wei Zhang
40 Xinglin Zhao
41 Xin Zhou
42 Qiang Zhu

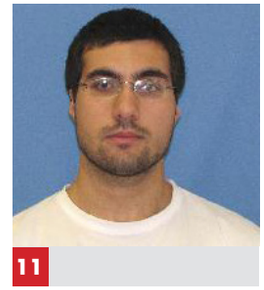


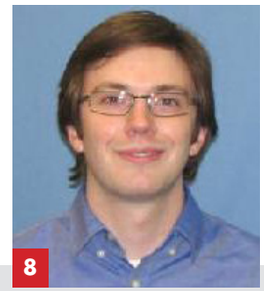


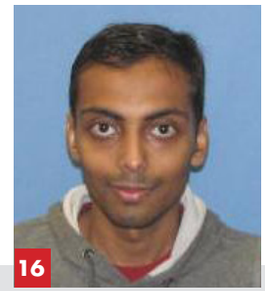










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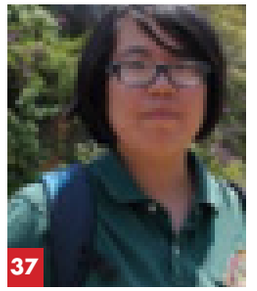
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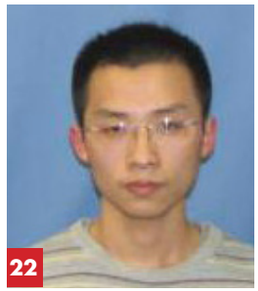
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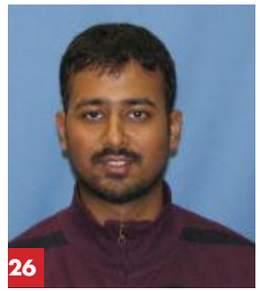
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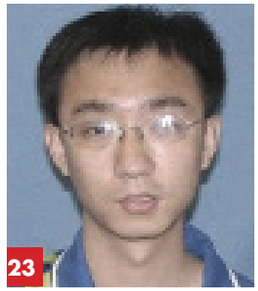
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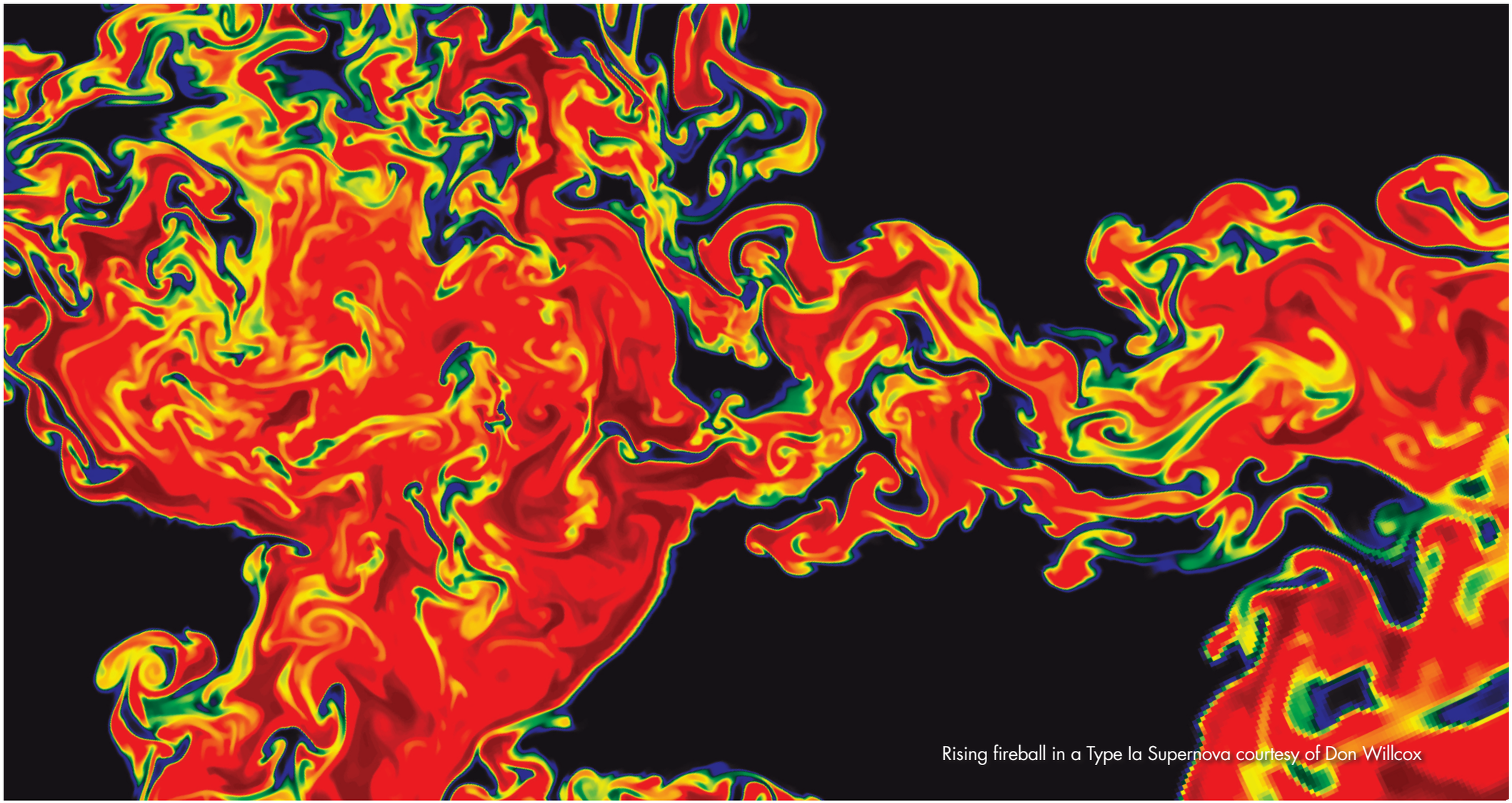

Rising fireball in a Type Ia Supernova courtesy of Don Willcox

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