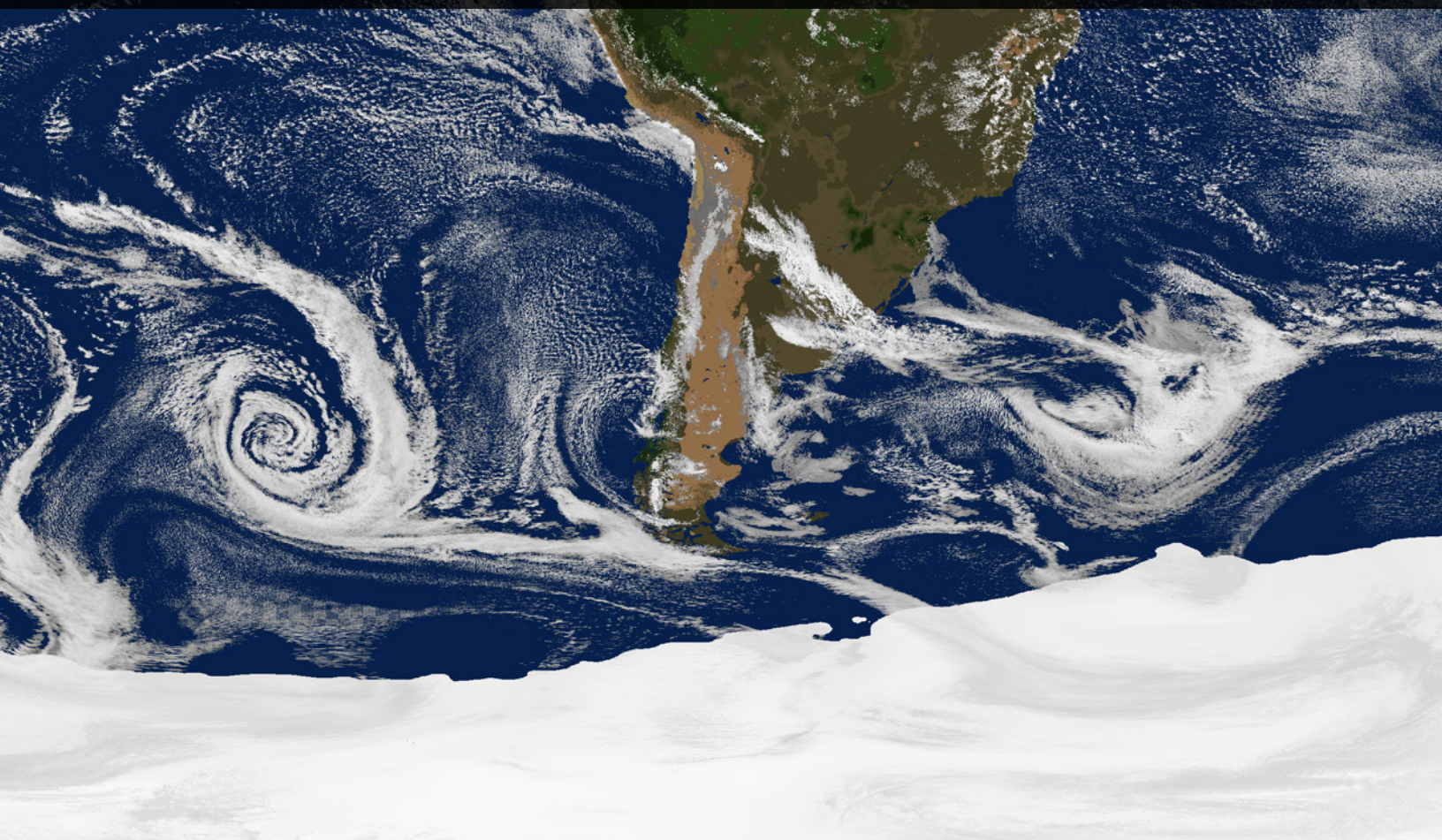


iACS

INSTITUTE FOR ADVANCED
COMPUTATIONAL SCIENCE

2018 ANNUAL REPORT



Message from the IACS Leadership Team

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As we wrap up our sixth year, we can feel proud of the well-oiled machine we call IACS that is providing a solid foundation for our future ventures to new frontiers in data and computational science and into new communities. We remain, however, always mindful of how lucky we are to have such outstanding and enthusiastic faculty and staff as well as the support of our gracious endowers. With their help, we continue to build on our past achievements, some of which are highlighted in the pages to come.

This year we welcome Bradley Spitzbart and Jessica Rojahn to our ranks. Bradley joined us in March as a Research Programmer with Professor Heather Lynch's group. He uses machine learning and high-performance computing to process and analyze large-scale satellite imagery. Jessica holds the newly-created position of IACS Social Media Representative. She has been instrumental in keeping the IACS social media sites up to date as well as creating new ways to get the word out about upcoming events and opportunities to all students and faculty.

On the recruiting front, we've made great progress in reaching out to the community. Our Diversity Coordinator Rosalia Davi arranged for six recruiting visits for IACS faculty and students to area colleges where we reached more than 150 prospective students, and we held our first virtual visit with Wofford College in South Carolina. Dr. Jennifer McCauley, who manages our STRIDE program, organized a trip for 32 high school girls from the local Hicksville School District to visit IACS and SBU, and our HS summer camp is still going strong, this year with an equal ratio of girls to boys.

Our faculty have also achieved important milestones and, in some cases, nationwide notability. Core faculty member Heather Lynch was featured on national TV and print media for her work with the Antarctic penguin population, and affiliate faculty Steve Skiena was named an AAAS fellow and the director of the new AI institute on campus.

Some additional highlights: Our pursuit of external funding continued this year with a record number of 40 proposals submitted for a total of almost \$45M funds requested: 16 proposals are still pending (valued at \$33M) and 14 were awarded (valued at \$4.35M).

Special thanks goes out to our departing Provost Michael Bernstein, who has been generous with his time and attention to all matters involving the institute. We also want to thank Interim Dean of the Graduate School Richard Gerrig who has helped us navigate the academic hurdles associated with our new certificate. As IACS affirms its role in the university, we have to also mention the support we've received from our department chairs, specifically Computer Science Chair Samir Das and Applied Mathematics and Statistics Chair Joseph Mitchell, who have both been instrumental in our endowed chair searches.

Sincerely,

Robert Harrison,
IACS Director

Alan Calder,
IACS Deputy Director

Lynn Allopenna,
IACS Administrative Director

VISION & MISSION

Vision

Our vision is to establish Stony Brook University at the forefront of data and computing in science and engineering by advancing vibrant interdisciplinary research and education programs, providing broad leadership across SBU and SUNY, and delivering demonstrated economic benefit to New York State.

Mission

To realize our vision, we will:

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

We presently have 13 core faculty spanning chemistry, materials by design, condensed matter, astrophysics, atmospheric science, nanoscience, linguistics, ecology, applied mathematics, and computer science. Another approximate 50 faculty are affiliated with the institute from diverse departments, and we are actively recruiting two endowed positions and two junior positions in computer science and applied mathematics.

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

IACS JR. RESEARCHER AWARD WINNERS FOR 2018



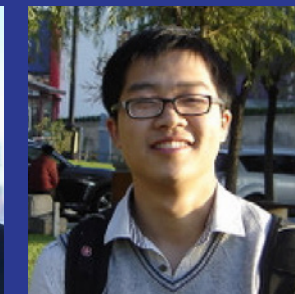
Alena Aksenova
Linguistics



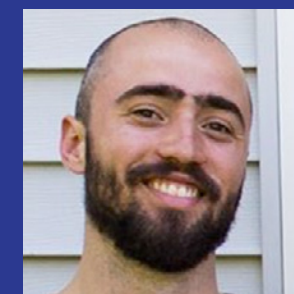
Jonathan Rawski
Linguistics



Bhavya Ghai
Computer Science



Junting Ye
Computer Science



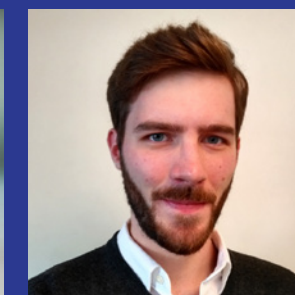
Bento Goncalves
Ecology and Evolution



Mikhail Ignatov
Applied Math and Statistics



Maria Barrios Sazo
Physics and Astronomy



Sebastian Dick
Physics and Astronomy

NEW AFFILIATES



Philip Armitage
Professor
Physics and Astronomy
Stony Brook University



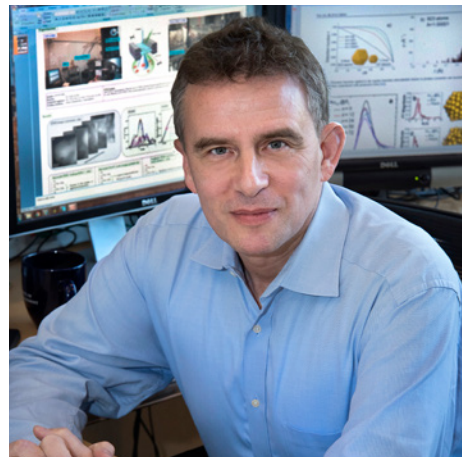
Mónica Bugallo
Professor
Electrical and Computer Engineering
Stony Brook University



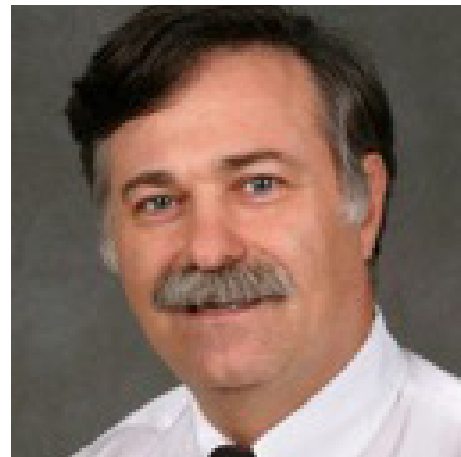
Brian Colle
Professor and Chair
School of Marine and Atmospheric Sciences
Stony Brook University



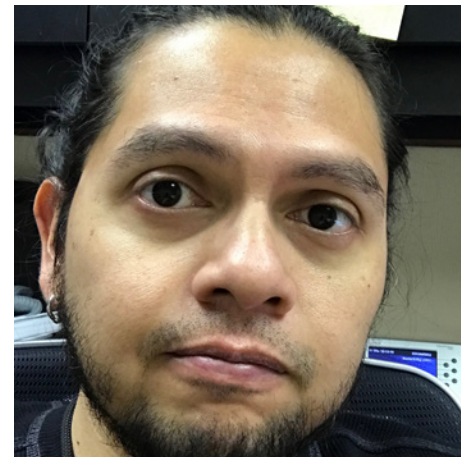
Sergey Syritsyn
Assistant Professor
Physics and Astronomy
Stony Brook University



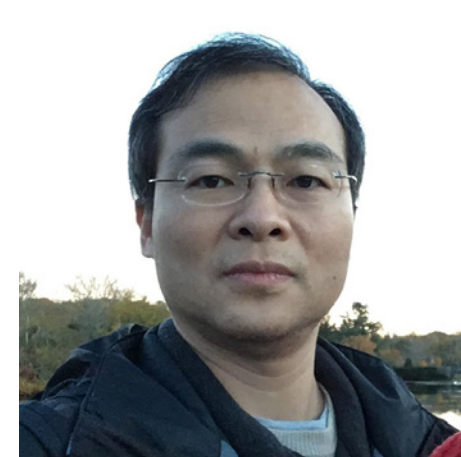
Anatoly Frenkel
Professor
Materials Science and Chemical Engineering
Stony Brook University



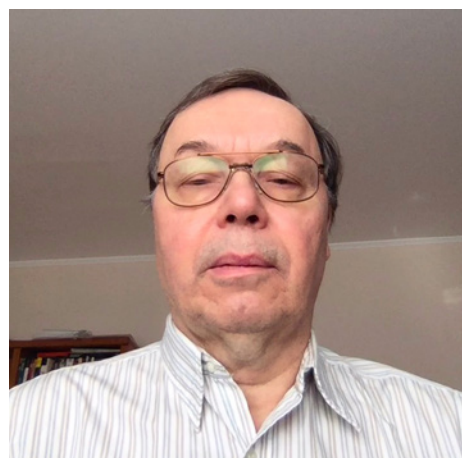
Arie Kaufman
Professor
Computer Science
Stony Brook University



Martin Kong
Assistant Computational Scientist
Computational Science Initiative
Brookhaven National Laboratory



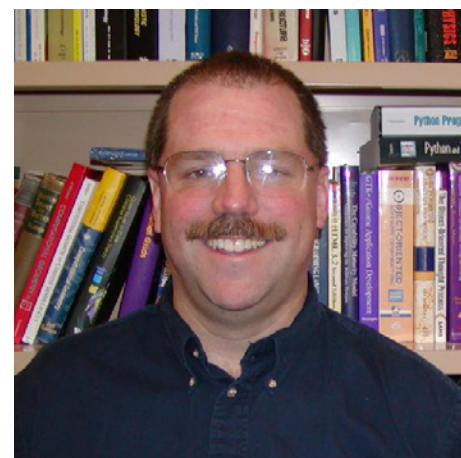
Tzu-Chieh Wei
Associate Professor
C.N. Yang Institute for Theoretical Physics
Stony Brook University



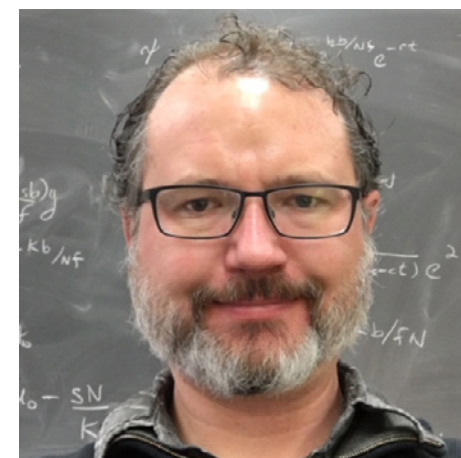
Vladimir Korepin
Professor
C.N. Yang Institute for Theoretical Physics
Stony Brook University



James Lattimer
Distinguished Professor
Physics and Astronomy
Stony Brook University



Douglas Swesty
Research Associate Professor
Physics and Astronomy
Stony Brook University



Christopher Wolfe
Assistant Professor
School of Marine and Atmospheric Sciences
Stony Brook University

NEW HIRES

Bradley Spitzbart joined IACS in March, 2018 as a Research Programmer with Associate Professor Heather Lynch's NSF funded ICEBERG program. He works with domain scientists in geology, ecology, and computer science to facilitate the open-source cyberinfrastructure necessary for the processing and analysis of large-scale satellite imagery using machine learning and high-performance computing resources.



Brad holds a BS in Mathematics from Valparaiso University and an MS in the Physical Sciences from the University of Chicago. Prior to coming to Stony Brook, he spent 16 years on the Science Operations Team with NASA's Chandra X-ray Observatory in Cambridge, MA.



Jessica Rojahn joined IACS in January, 2018 as a front desk Graduate Assistant. In September, she took on the extra duties associated with the newly created position of IACS Social Media Representative. Wearing her other hat as a PhD candidate in the Sociology Department, she has her finger on the pulse of the graduate student population at SBU and can therefore effectively spread IACS'

message and opportunities to more departments and students than ever before. She has already made great strides leading IACS to new frontiers to connect and share with others the great news and opportunities available through the institute.

SEMINARS & PROGRAMS

IACS Seminar Series

January 25, 2018

Suresh Venkatasubramanian, University of Utah

Algorithmic Fairness: Doing Good (or at Least Doing No Harm) with Automated Decision-making

January 26, 2018

Henri Calandra, Total Paris, France

Transition to Exascale, a User Perspective

January 26, 2018

Serge G. Petiton, University of Lille

Toward Computational and Data High Performance Intelligent Methods for Extreme Scale Distributed and Parallel Hypercomputers

February 1, 2018

Alan Calder, Stony Brook University

Capturing the Fire: Flames and Flame Models in Astrophysics

February 15, 2018

Gary King, Harvard University

How to Measure Legislative District Compactness if You Only Know It When You See It

April 12, 2018

Jonathan Dursi, Toronto's Hospital For Sick Children

Dispatches from the Convergence Coalface: HPC, Big Data, and Large Scale Genomics

April 26, 2018

Ignacio Franco, University Of Rochester

Challenges in the Atomistic Modeling of Nanoscale Junctions: Lasers, Forces, Statistics and Beyond

May 4, 2018

Tzu-Chieh Wei, Stony Brook University

Introduction to Quantum Computation: What's All the Fuss About?

August 30, 2018

Misha Chertkov, Los Alamos National Laboratory

Interpretable and Tractable Machine Learning for Natural and Engineering Sciences

September 13, 2018

Mehryar Mohri, New York University

Competing with Weighted Automata Experts

September 26, 2018

Mark Squillante, IBM

Optimization under Uncertainty

September 27, 2018

Eric Winsberg, University of South Florida

Tuning Models for Skill: When is Prediction Better than Accommodation?

September 27, 2018

Rose McCallen, Brian Weston, Lawrence Livermore National Laboratory

Science and Engineering R & D Challenges at a DOE National Laboratory

October 4, 2018

Alexander Orlov, Stony Brook University

Exploring New Catalytic Materials on Nanoscale: Novel Methods of Synthesis, Characterization and Computational Needs

October 12, 2018

Brian Wirth, University of Tennessee Knoxville and Oak Ridge National Laboratory

Overview of Modeling Plasma Surface Interactions in Tungsten with a Focus on Connecting Computational Predictions to Experimental Observations

October 18, 2018

Sommer Gentry, United States Naval Academy

Liver Transplant Equity: Simplify, Optimize, Simulate, Scrutinize

October 25, 2018

Rainer Engelken, Columbia University

A Dynamical Systems Perspective on the Controllability Chaotic Neural Circuits

November 8, 2018

Katy Huff, University of Illinois at Urbana-Champaign

Doing Our Best: Approaches in Scientific Computing

November 9, 2018

Dmitri Kharzeev, Stony Brook University

Chiral Magnetic Effect in Dirac and Weyl Semimetals: Towards the Chiral Qubit

November 12, 2018

Ryan Cotterell, Johns Hopkins University

Probabilistic Typology: Deep Generative Models of Vowel Inventories

November 13, 2018

Cody Buntain, New York University

Scalable Methods for Increasing Recall and Precision in Social Media Datasets

December 7, 2018

Dominik Schneble, Stony Brook University

Quantum Simulations with Ultracold Atoms in Optical Lattices



Projects, Programs, and Events

Python Programming Workshop

January 18, 2018

IACS Bootcamp: R Programming for Beginners

January 20, 2018

NACLO - North American Computational Linguistics Olympiad at Stony Brook University

January 25, 2018

IACS Bootcamp: R Programming for Beginners #2

January 27, 2018

Become a Software Carpentry Instructor

January 30, 2018

XSEDE HPC Workshop: Big Data

February 7, 2018

Tutorial Workshop: Big Data Analytics Without Fast Data Compromises

March 1, 2018

IACS Google Cloud Workshop

March 12, 2018

IACS Research Day 2018

April 4, 2018

NowNet Arts Conference 2018

April 19, 2018

IACS Open House for Advanced Graduate Certificate in Data and Computational Science

May 3, 2018

Joint Science Meeting

May 21, 2018

New York Scientific Data Summit (NYSDS) Data-Driven Discovery in Science and Industry 2018

August 6, 2018

XSEDE HPC Workshop: OpenMP

August 7, 2018

HPC Workshop: "SeaWulf Basics"

September 27, 2018

XSEDE HPC Workshop: MPI

October 2, 2018

IACS Information Session

October 11, 2018

IACS Bootcamp: Intro to R Programming

October 22, 2018

CNC 2018: The Tenth Annual Concurrent Collections Workshop

November 29, 2018

SeaWulf HPC Training Workshop

December 6, 2018



HPC Users Reach Record Numbers

The team enjoys an end-of-semester night out on the town. L-R: Senior HPC Engineer Eric Rosenberg, Benjamin Yu, Janet Vorobyeva, David Carlson, Ibironke Osipitan, alumnus Tyler Estro, Christian Arty, Anand Aiyer, and Jesse Talavera-Greenberg.

Support team keeps up with the challenging pace

This year the HPC Support Team earned its keep by helping approximately 580 users of SeaWulf, the university's 164-compute node system dedicated to research computing on campus. (This number has more than doubled from 263 users last year.) Special recognition goes to Senior HPC Engineers Eric Rosenberg and Firat Coskun who oversaw the merge of SeaWulf with LI-red, a 100-compute node cluster funded by the Long Island Regional Economic Development Council. In March of 2018, the two clusters were merged into a single high-performance cluster in order to provide a more straightforward and seamless user experience for Stony Brook researchers. In total, the Stony Brook University computing clusters include 264 nodes and 6,992 cores, with a peak performance of ~ 340 TFLOP/s available for research computation.

The team of students who work behind the scenes and are the backbone of HPC Support are a mix of undergraduates and graduates. Last year's crew saw the return of all but four students. The returning team members are Ecology and Evolution PhD student David Carlson; Computer Science PhD student Ruhul Amin; Applied Mathematics PhD student Ruyi Yu; Computer Science Master's student Jesse Talavera-Greenberg; and Computer Science undergraduates Ibironke Osipitan and Janet Vorobyeva.

To keep the support team functioning at peak performance, three new students were hired into the group this year. Support for HPC resources receives "good marks" from faculty and student users, and proposals for new advanced hardware are in the works. With the strong support of the team, the future for HPC at SBU is bright.

HPC STATS

NUMBER OF SEAWULF USERS:

580

NUMBER OF DEPARTMENTS REPRESENTED BY USERS:

38

NUMBER OF CLASSES:

8

CLASSES TAUGHT USING SEAWULF IN 2018:

CSE 628 Natural Language Processing

EBH 381 Genomics Laboratory

AMS 536 Molecular Modeling of Biological Molecules

AMS 530 Principles in Parallel Computing

AMS 598 Big Data Analysis

CSE 504 Compiler Design

PSY 610 Micro Imaging Laboratory

SOC 591 Computational Social Science

Anand Aiyer

Anand is a third year PhD student in Computer Science specializing in Artificial Intelligence. At HPC Support, he works with researchers in Biomedical Informatics and Computer Science who employ the latest machine learning techniques in Computer Vision for Digital Pathology and Cancer Research. He is the go-to resource for researchers interested in learning how to leverage the power of Deep Learning for projects using SeaWulf.

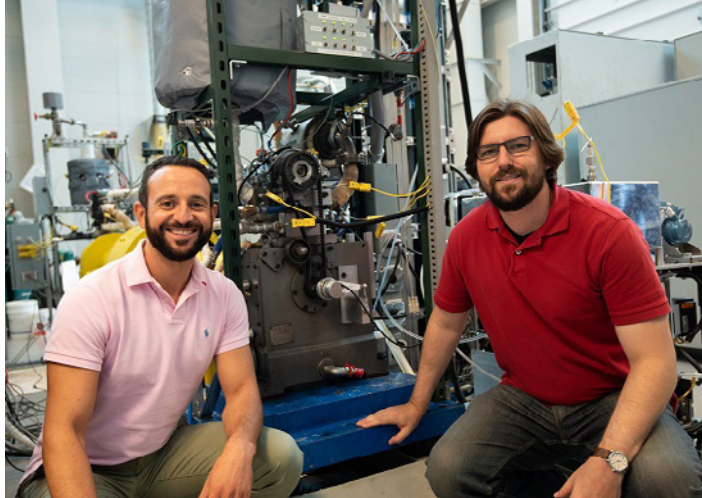
Benjamin Yu

Benjamin is a senior studying computer science. He has been improving the system environment on SeaWulf by developing unit tests to automate software maintenance of dozens of programs such as MatLab and Mathematica. Furthermore, he has contributed to the workflow of many users through converting projects to run in parallel and resolving customer service tickets through troubleshooting and debugging system issues.

Christian Arty

Christian is a senior majoring in biology and minoring in chemistry. He has been continuously improving various aspects of SeaWulf through performing maintenance and hardware upgrades, as well as through introducing new software packages, such as CRYO-EM, for research groups. Additionally, he assists the Biomedical Informatics Department with different machine learning projects that facilitate the progression of digital pathology. He specializes in Python, utilizing his skills to provide technical support for SeaWulf users with their projects.

SeaWulf was made possible by a National Science Foundation grant (#1531492). Support for the HPC student team is made possible by the Division of Information Technology, headed by Senior Vice President for Information Technology and Chief Information Officer Dr. Melissa Woo. Any faculty member interested in using the cluster, or having the cluster available for his/her research group, can request a project number through SBU's online ticketing system accessed here: <https://it.stonybrook.edu/help/kb/getting-a-project-on-seawulf-or-li-red>.



Reprinted with Permission from the College of Engineering and Applied Sciences

The College of Engineering and Applied Sciences announces that Professors Sotirios Mamalis and Ben Lawler in the Department of Mechanical Engineering (<https://me.stonybrook.edu/>) have received a \$1.49 million grant from the U.S. Department of Energy (DOE) - Vehicle Technologies Office. Their proposal, "Naphthenic Biofuel-Diesel Blend for Optimizing Mixing Controlled Compression Ignition Combustion," was selected as part of a total of \$10.1 million in funding to Engines and Fuels research projects.

"Our research will advance the state-of-the-art of biofuels by introducing a new naphthenic blend produced from loblolly pine," said Sotirios Mamalis, assistant professor of mechanical engineering and the principal investigator (PI) for the project. "It will also provide a detailed set of experimental data showing the effects of the biofuel addition on diesel engine combustion and help identify the next generation of biofuels that can pave the way towards carbon neutral transportation."

"This research will help invent technologies that promote energy efficiency and environmental sustainability with the potential to impact the future of transportation fuels, while offering significant benefits through reduction in greenhouse gases and improved air quality," said Fotis Sotiropoulos, Dean, College of Engineering and Applied Sciences (<https://www.stonybrook.edu/ceas/>). "Sotirios and Ben are relentless in their pursuit of new technologies that offer alternatives to traditional fuels and combustion. I applaud their efforts and look forward to the outcomes of their research."

This project is focused on developing and testing a new biofuel that can be used in current and future diesel engines, to displace petroleum-derived fuel and reduce greenhouse gas emissions from transportation and power generation. Unlike existing biofuels that are largely derived from food crops, the proposed biofuel is derived from loblolly pine, which makes it more economically attractive. Stony Brook has partnered with RTI International (North Carolina <https://www.rti.org/>), a non-profit research organization, which will investigate the production and upscale of the new biofuel. Stony Brook University will evaluate the biofuel's chemical properties, and test it in a research engine to assess its performance compared to conventional diesel fuel. The project team will also analyze the lifecycle of the new biofuel, including production and

ADVANCING BIOFUELS FOR TRANSPORTATION AND POWER GENERATION WITH \$1.49 MILLION DOE AWARD

combustion in the engine, to quantify the greenhouse gas reductions that it can offer compared to petroleum-derived fuels. Throughout the execution of this project, the team will work with a group from the DOE National Laboratories (<https://www.energy.gov/national-laboratories>) that is focused on developing advanced biofuels for future internal combustion engines. The project will be conducted over a period of three years.

The award is among 42 projects totaling \$80 million selected for funding by the DOE to support advanced vehicle technologies that can enable more affordable mobility, strengthen domestic energy security, reduce the U.S. dependence on foreign sources of critical materials, and enhance U.S. economic growth. This work supports DOE's goal to invest in early-stage research of transportation technologies that can give families and businesses greater choice in how they meet their mobility needs.

DOE press release: Department of Energy Announces \$80 Million investment in Advanced Vehicle Technologies Research (<https://www.energy.gov/articles/department-energy-announces-80-million-investment-advanced-vehicle-technologies-research>)

ABOUT THE RESEARCHERS:

Sotirios Mamalis (PI) is an assistant professor in the Department of Mechanical Engineering and an affiliate member of Stony Brook's Institute for Advanced Computational Science (IACS <https://iacs.stonybrook.edu/>). His research is in power generation and propulsion systems with emphasis on internal combustion engines using conventional and alternative fuels. He joined the Stony Brook faculty in 2013 and holds a PhD in mechanical engineering from the University of Michigan. Visit his research lab's page at: Engine Combustion Research (<https://you.stonybrook.edu/combustion/>).

Benjamin Lawler (Co-PI) is an assistant professor in the Department of Mechanical Engineering. His research is focused on improving the efficiency and emissions of internal combustion engines, including the use of alternative fuels or advanced combustion concepts. He joined the Stony Brook faculty in 2015, and received a PhD in mechanical engineering from the University of Michigan. Visit his research lab's page at: Engine Combustion Research (<https://you.stonybrook.edu/combustion/>).

NowNet Arts Conference @ SBU

"Network Music: Artistic and Technological Strategies for Public and Private Networks" took place April 19-22 at IACS with 30 remote locations internationally. Participants attended in-person and online via conferencing and webstream.

Network Music utilizes the internet as a contemporary artistic medium for musicians on both localized networks and geographically spatialized networks. Network Music has proliferated in recent decades in forms for live performance such as telematic ensembles, laptop ensembles, virtual world collaborations, and multidisciplinary work. Artists and technologists in this medium have utilized Internet2 and its international partner networks to achieve live concert-quality productions locally and globally, especially requiring the high-bandwidth and quality of service provided by these networks. Internet2 and its partners are largely available at large research universities so the medium has remained mostly in this research sphere. With the rise of availability of high-bandwidth public networks, Network Music is at a juncture where the medium can become more accessible to the public through a wider range of universities and contemporary arts venues, while the advancements of Internet2 and its partners continue to provide state-of-the-art opportunities to artists and technologists.

Through the papers, workshops, presentations, and concert demonstrations the conference was able to establish proof-of-concept in connecting with both public and private networks, utilizing a variety of technologies on different bandwidths and system configurations, and working across disparate venue spaces, while innovating artistic applications for the medium. The results created a new paradigm of high-level strategies for continued utilization of Internet2 in the medium while opening the field wider to use of public networks in collaboration. As a first-of-a-kind conference on this topic, NowNet Arts will continue expanding and applying this work in future programs.



Joint Science Meeting participants gathered for dinner one night during the conference.

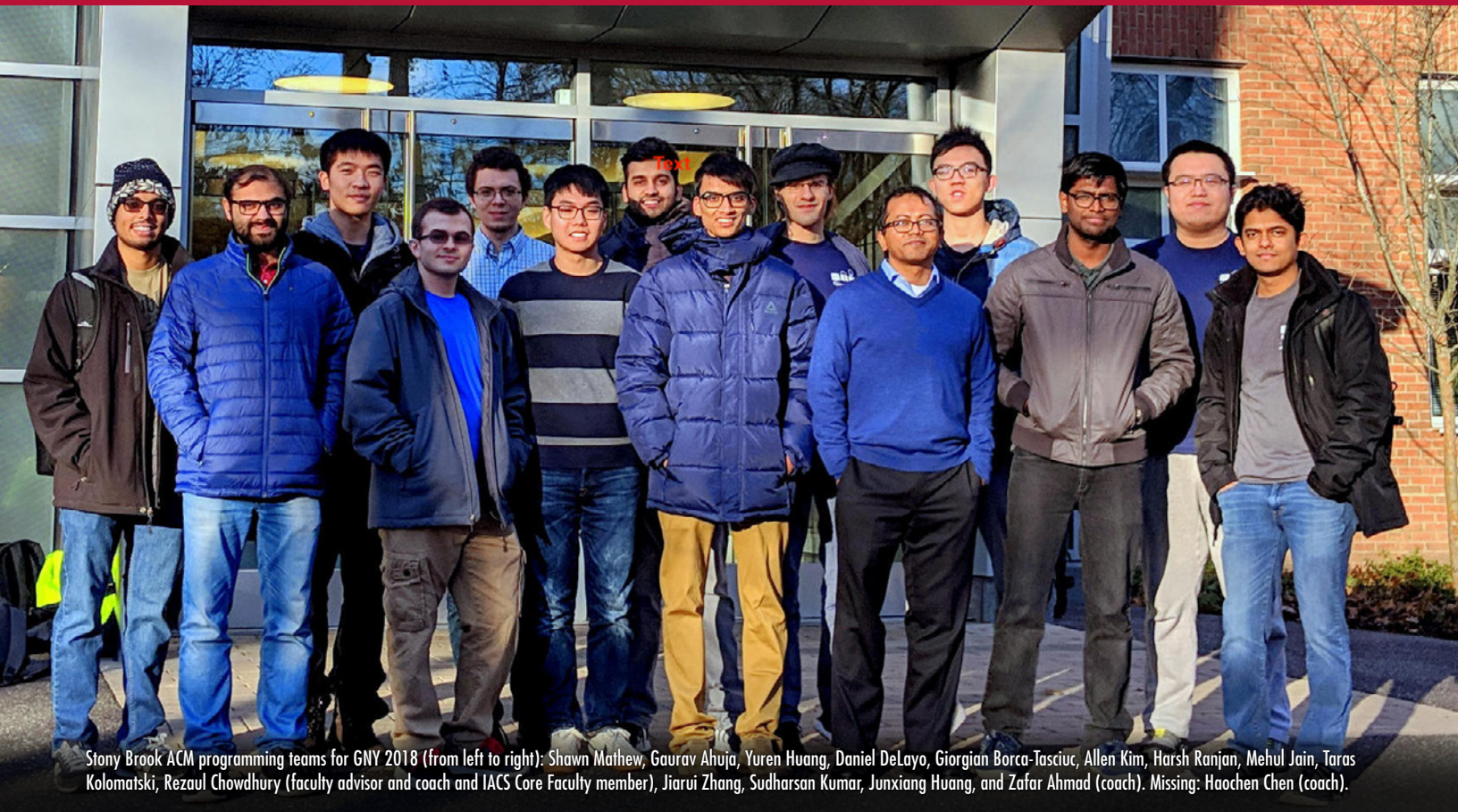
JOINT SCIENCE MEETING

Over 65 participants from the Tokyo Institute of Technology (TIT), Brookhaven National Laboratory (BNL), and SBU attended the IACS Joint Science Meeting held on campus May 21-23. The 3-day workshop was an opportunity for IACS faculty and students to share their knowledge and passion and to identify and develop new opportunities for collaboration

with their Japanese colleagues. Keynotes and contributor talks were centered on five topics of mutual interest: Quantum Computing; Physics: Small and Large Experiments; Materials Science Condensed Matter/Chemistry; HPC/Big Data; and Environmental Science and/or Engineering.

In addition to the keynotes and contributor talks, attendees participated in themed breakout lunch sessions, a cocktail reception and poster session, and a sit-down dinner at the Wang Center. The meeting served as the central enabling activity of the partnership between the Tokyo Institute of Technology and Stony Brook University to pursue common interests in science, engineering, technology, and especially the education and preparation of students.





Stony Brook ACM programming teams for GNY 2018 (from left to right): Shawn Mathew, Gaurav Ahuja, Yuren Huang, Daniel DeLayo, Georgian Borca-Tasciuc, Allen Kim, Harsh Ranjan, Mehul Jain, Taras Kolomatski, Rezaul Chowdhury (faculty advisor and coach and IACS Core Faculty member), Jiarui Zhang, Sudharsan Kumar, Junxiang Huang, and Zafar Ahmad (coach). Missing: Haochen Chen (coach).

IACS Faculty helps SBU's CE CS Math Team place 4th in ACM Greater NY Regional Programming Contest

Stony Brook's top team consisting of students from Computer Engineering, Computer Science, and Mathematics finished 4th in the 2018 ACM ICPC Greater New York Regional Programming Contest held at Manhattan College on November 19, 2018. They finished behind one team from Columbia, Princeton, and Cornell each and ahead of everyone else including the remaining teams from Princeton (3 teams), Cornell (4 teams), Yale (3 teams), Columbia (1 team), NYU (4 teams), Rochester (1 team), and Rutgers (3 teams). Stony Brook's other teams were ranked 20th, 26th, and 37th among 68 participating teams.

Rank	Name	Solved	Time	A	B	C	D	E	F	G	H	I	J	Total att/solv
1	Columbia - Kington	8	893	1/13	0/--	1/119	1/205	2/47	1/81	1/139	1/65	0/--	2/184	10/8
2	Princeton 1	8	1185	1/5	0/--	1/75	1/246	7/195	2/67	1/203	1/102	0/--	1/152	15/8
3	Cornell i*2	7	830	1/12	1/--	1/98	0/--	1/175	1/133	1/213	1/57	0/--	1/142	8/7
4	SBU-Ereshkigal	7	919	2/9	6/--	1/103	0/--	5/217	1/106	1/81	3/110	0/--	1/173	20/7
5	Princeton 3	7	993	1/6	0/--	1/162	0/--	1/186	1/103	1/211	1/43	0/--	1/282	7/7
6	Rochester 1	7	1147	1/6	2/--	2/82	4/--	6/121	7/241	1/140	1/54	0/--	1/263	25/7
7	Princeton 2	6	994	1/7	0/--	1/76	0/--	5/241	1/154	0/--	2/117	0/--	1/299	11/6
8	NYU HuaNong Brothers	6	1127	1/10	0/--	1/233	0/--	4/221	3/181	1/--	1/83	0/--	1/299	12/6
9	Cooper Union 1	6	1142	1/9	0/--	1/217	0/--	8/268	1/36	2/178	2/254	0/--	0/--	15/6
10	NYU Small Transparent	5	652	1/9	0/--	1/128	0/--	4/181	1/98	0/--	1/176	0/--	0/--	8/5
11	Cornell 5	5	736	1/6	0/--	2/175	0/--	2/98	2/--	0/--	1/139	0/--	1/278	9/5
12	NYU TooYoung	5	749	1/12	0/--	2/119	0/--	2/144	3/--	4/--	1/148	0/--	1/286	14/5
13	Rutgers Scarlet Pyrotechnics	5	963	1/14	0/--	1/199	0/--	2/186	1/287	0/--	1/257	0/--	0/--	6/5
14	Princeton 4	4	395	1/46	0/--	1/78	7/--	4/--	1/152	0/--	1/119	0/--	0/--	15/4
15	Yale 3	4	521	1/14	0/--	2/154	0/--	3/--	3/--	0/--	1/61	0/--	1/272	11/4
16	Yale 2	4	573	2/23	0/--	1/199	0/--	3/--	1/249	1/--	1/82	0/--	0/--	9/4
17	Cornell AHP	4	642	2/28	0/--	1/259	0/--	2/--	1/109	0/--	1/226	0/--	0/--	7/4
18	NYU A Team	4	656	5/62	0/--	0/--	0/--	5/299	0/--	3/--	1/46	0/--	1/109	15/4
19	Cornell 666	4	694	4/43	0/--	1/275	0/--	2/170	0/--	0/--	2/106	0/--	0/--	9/4
20	SBU-Artemis	4	712	2/13	0/--	1/218	0/--	0/--	0/--	0/--	2/161	0/--	1/280	6/4

The final rank list of the top 20 teams is given at right.

SBU teams are highlighted.



IACS Faculty wins AI for Earth award

Heather Lynch and ten others win Microsoft and Nat'l Geographic Society grants

IACS core faculty member and Ecology and Evolution Associate Professor Heather Lynch applied for a grant last July from a joint program involving a partnership between Microsoft and National Geographic Society. The grant was aimed at researchers who use Artificial Intelligence (AI) to tackle the world's critical environmental challenges. Winners were announced this week, and under the category of biodiversity conservation was our own Heather Lynch, who has teamed up with Dimitris Samaras, from Stony Brook's Computer Science Department, to develop AI-based algorithms for tracking penguins from satellite imagery.

"I've been manually annotating imagery for nearly a decade," says Lynch, "but the work is so labor intensive that it's just not a good solution for regular monitoring across the entire Antarctic. Teaming up with Dimitris Samaras and his students has opened an exciting new chapter in penguin conservation - their expertise in computer vision is clearly where the field needs to go, and I'm delighted that this new grant will allow us to plow ahead with this exciting interdisciplinary work."

Heather tracks Antarctic penguin populations to forecast the impacts of climate change. She uses satellite imagery to find guano stains, which are indications of the penguins' whereabouts and their population estimates. Winning this award will not only fund two graduate students in Computer Science, but it also provides for considerable computing support through Microsoft Azure. "Automated algorithms for penguin detection may be labor saving from a human perspective, but this remains computationally-intensive work, and the support from Microsoft will be absolutely key as we work to scale up a sustainable solution for penguin conservation," notes Lynch.

In addition to winning this prestigious grant, earlier in the year Professor Lynch was featured on national and international media including The NY Times, The Wall Street Journal, CBS News, Canada's CTV News, and the BBC, for discovering a major hotspot of penguin abundance in the Danger Islands Antarctica. Using satellite imagery not previously known to exist, she collaborated with several other institutions to lead the first ever expedition to the region, where they used drones and direct manual counting to complete the first complete survey of the region. Through subsequent analysis of the data, which involved developing machine learning algorithms to count penguins in drone imagery, it was confirmed that this region was a major hotspot of penguin abundance, including two of the world's largest colonies of Adélie penguins, and contained in total more than 50% of all the Adélie penguins in the Atlantic sector of the Antarctic.

IACS Affiliate Steven Skiena named AAAS Fellow 2018

Distinguished Teaching Professor Steven Skiena, from the Department of Computer Science and Director of the Institute for AI-Driven Discovery and Innovation in the College of Engineering and Applied Sciences, was named a fellow in the AAAS Section on Information, Computing and Communications for distinguished contributions to the fields of algorithms and data science, particularly interdisciplinary work in the biological and social sciences.

"I am greatly honored to be named an AAAS fellow, particularly to be joining the list of Stony Brook's previous AAAS fellows displayed in the Melville Library," said Skiena.



Science Training and Research to Inform DEcisions (STRIDE) Closes Out A Successful Second Year

STRIDE continues to bring exciting opportunities to STEM graduate students at Stony Brook University. The NSF-funded training program expanded this year to include Stony Brook's Public Health department and its respective faculty member Professor Jaymie Meliker. Other new faculty participants include Profs. Zhenhua Liu from Applied Mathematics and Statistics (AMS) and Laura Wehrmann from the School of Marine and Atmospheric Sciences (SoMAS).

FELLOWS

STRIDE awarded fellowships this year to Rachael Herman, Julia Stepanuk, Kristjan Mets, and Lisa Prowant from Ecology & Evolution (E&E), Adelle Molina, Stephen Tomasetti, Tara Dolan, Lisa Herbert, and Kylie Langlois from SoMAS, Zahraa Krayem from Electrical and Computer Engineering, and Joshua Comden from AMS. STRIDE fellows receive full tuition reimbursement, including registration fees and a \$200 textbook allowance, plus health benefits and a \$34,000 annual stipend.

C-STRIDE

Students enrolled in the C-STRIDE 15-credit certificate program are required to register for the Computer Science course titled Visualization. This fall was the first run of this course that included STRIDE students. In preparation for the



course, IACS offered a 2-day boot camp just prior to the beginning of the semester on Python for STRIDE trainees. With the support of Professor Klaus Mueller and several specialized teaching assistants, STRIDE trainees were better prepared to tackle the demands of the Visualization course, which is core to the certificate.

EVENTS

STRIDE-Con is a day-long event that showcases talks on science communication, data visualization, and policy. Professor Christine O'Connell gave a talk focusing on how to challenge stereotypes while cultivating diverse voices in science communication, and Professor Thomas Woodson presented a talk highlighting the inextricable links between science and policy. The day's plenary speaker was Dr. Brian Zikmund-Fisher of the School of Public Health at the University of Michigan who offered thoughtful insights on aiding the decision-support process, particularly with regard to deciding



which data to emphasize to a particular audience.

At the close of the day, *STRIDE-Con* held its second annual visualization contest, which is open to all graduate students. The winning figure was submitted by Jessica Maghakian (AMS) entitled Detecting Gerrymandering: A Data-Driven Look at the US Congressional Districts from 2003-2013. Jessica won an all-expense paid trip to the renowned Edward Tufte visualization workshop.

Many Paths to Science involved scientists from various fields in a panel setting discussing their personal career trajectories and giving advice to future PhDs, focusing this year on consulting and entrepreneurship. Panelists included STRIDE's own Prof. Erez Zadok, who is experienced with small-business and consulting; Dr. Deb Aronson, Director of Medical Strategy at Intouch Solutions and an energetic and self-professed outspoken science blogger with various startups focusing on science communication; Dr. Mehdi Namazi, a postdoctoral fellow at Yale University and the co-founder and CEO of Qunnect, LLC; and SBU alum Dr. Tomasz Bakowski, a life sciences strategy consultant at Acel Health, a boutique science consulting firm.

Throughout the year, there were monthly *Brown Bag Lunches* open to everyone on campus. Topics ranged from technical advice with navigating Adobe Illustrator to designing an effective résumé and cover letter to learning about science policy from Kei Koizumi, a former Assistant Director for Federal Research and Development and chief advisor on science and technology budgets during the Obama Administration.

In addition, this year STRIDE rolled out a new and exciting program entitled *Pizza & Policy*, where students and faculty gather to discuss science policy or a particular piece of legislature while enjoying a pizza lunch.



An important milestone for STRIDE in 2018 was graduating the program's first alumnus, Dr. Xin Zhou. Dr. Zhou completed his PhD in atmospheric sciences along with the advanced graduate certificate C-STRIDE, and is now a postdoctoral fellow at Brookhaven National Laboratory (BNL). He attributes securing his position at BNL as the result of a very successful internship while he was still a student that was arranged by STRIDE. Dr. Zhou also cites his experiences with STRIDE as helping him to better engage with his colleagues and research team.

COMMUNITY OUTREACH

STRIDE continues to move forward with its goal of making STEM education more diverse and inclusive. With this pursuit in mind, STRIDE faculty, staff, and trainees went on several recruiting trips to colleges and universities that have large underrepresented populations including the College of New Rochelle; Morgan State University; CUNY John Jay; and University of Maryland: Baltimore County.

Likewise, in the pursuit of making STEM more equitable for all, STRIDE participated in several K-12 Education outreach opportunities, most recently hosting 32 young women from Hicksville High School for a "Women in STEM Day," wherein participants enjoyed talks by women STEM faculty, women graduate students, and a hands-on project in Electrical & Computer Engineering led by STRIDE graduate student Zahraa Krayem.

NAME RECOGNITION MOVED TO THE FOREFRONT AT IACS

Four research themes are developed to help brand the institute

Four initial research themes have been developed after an extensive and ultimately very enjoyable discussion that attracted broad engagement from our core and affiliate faculty. The purposes of the themes are to focus the institute's attention on current and high-impact multidisciplinary research topics; to create new collaborations; to engage and motivate our students; and to develop name recognition. Some recurring questions the IACS Advisory Board has been asking of the institute's leadership are: what makes IACS unique; how does the institute want to be recognized nationally and internationally; what is our identity; and how do we brand ourselves to stand apart from others in the field. Going forward, we will align many of our research investments with the themes that are also a central part of our plans for growth. This starts immediately with our seminar program – by having themes host speakers we strive for broader benefit and stronger participation at events. Each IACS faculty member has identified one or more themes in which they will participate.

Each group has created a Slack channel to communicate ideas and collaboratively work on proposals; each group invites one external speaker per semester to talk about the relevant research going on elsewhere in the world; and each group conducts a slate of regular meetings to discuss how best to move their themes forward. For anyone who has an interest in any and all of these groups, you are encouraged to reach out to the theme leaders and request to join. For more information, you can visit <https://iacs.stonybrook.edu/research/index.php>.

Machine Learning and Statistical Inference for Scientific Discovery

(Participants in alphabetic order with leaders in bold)

Jeffrey Heinz	Predrag Krstic	Steven Skiena
Heather Lynch	Sotirios Mamalis	Jason Trelewicz
Barbara Chapman	Klaus Mueller	Song Wu
Rezaul Chowdhury	I. Memming Park	Shinjae Yoo
Thomas Graf	Matthew Reuter	Minghua Zhang
Xiangmin Jiao	Roy Shilkrot	Mike Zingale
Jason J. Jones	Hideo Sekino	
Dima Kozakov	Carlos Simmerling	

This highly-active group advances the state-of-the-art in the techniques and applications of machine learning and statistical inference to explore frontiers in scientific discovery. Researchers develop and apply methods in supervised and unsupervised machine learning techniques ranging from deep learning to statistical and computational learning theories to Bayesian data analysis to other paradigms of statistical inference and beyond for hypothesis generation, testing, and evaluation.

High-performance Computing and Future Computing Technologies

Robert Harrison	Jason J. Jones	Hideo Sekino
Barbara Chapman	Dima Kozakov	Jason Trelewicz
Rezaul Chowdhury	Predrag Krstic	Shinjae Yoo
Dilip Gersappe	Meifeng Lin	Minghua Zhang
Jeff Heinz	Heather Lynch	
Xiangmin Jiao	Sotirios Mamalis	

This group advances the art and practice of scientific computation and data spanning laptops to exascale supercomputers to future quantum and other technologies. Research includes programming models and runtime systems; advanced numerical methods and fast algorithms; HPC for scientific discovery and engineering design; effective use of exascale computer systems; integrating ML and HPC into applications; cloud and data-centric computation for science and education; and scientific reproducibility and uncertainty quantification. The group is interested in the development and effective use of future computer technologies including quantum computing and information theory; neuromorphic processors; FPGAs; data-centric systems; and network topologies.

Simulation, Modeling, and Analysis of Complex Systems

Jason Trelewicz	Predrag Krstic	Shinjae Yoo
Frank Alexander	Meifeng Lin	Minghua Zhang
Rezaul Chowdhury	Janet Nye	
Dilip Gersappe	I. Memming Park	
Xiangmin Jiao	Matthew Reuter	
Jason J. Jones	Hideo Sekino	
Dima Kozakov	Carlos Simmerling	

This group studies deterministic and stochastic systems to understand interactions between components and the emergence of system-wide behavior. The computational analyses are validated with experimental data and also often identify mechanisms that relate model parameters and observables. In addition to application domains, the current research themes include multi-scale modeling, scientific reproducibility, and uncertainty quantification.

Making Sense of Data

Meg Schedel	Heather Lynch	Steven Skiena
Liliana Dávalos	Klaus Mueller	Shinjae Yoo
Rezaul Chowdhury	Alexander Orlov	Minghua Zhang
Jeff Heinz	I. Memming Park	Mike Zingale
Marat Khairoutdinov	Hideo Sekino	
Predrag Krstic	Roy Shilkrot	

Led by faculty from the Music Department, this group makes data easier to understand and communicate by developing and applying tools and techniques to find structures in complex datasets, and by engaging with data using all of our senses. Using a combination of data science including data analytics, intelligent computing, and machine learning, coupled with an understanding of human cognition, perception and ergonomics, the group will verify, disprove, and explain scientific models, theories and hypotheses. They will communicate their results through integrative quantitative data analysis as well as qualitative interpretations such as scientific visualizations, sonifications, and extended reality (XR) displays.

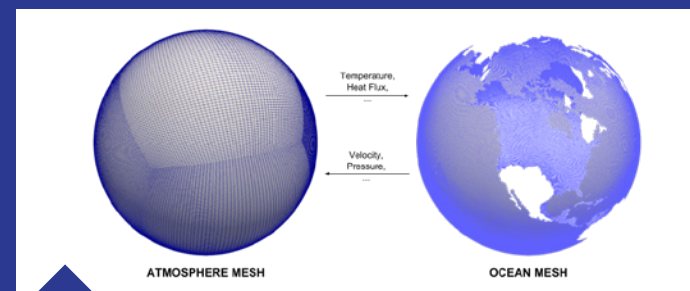


Participants in the POLAR 2018 conference held in Davos, Switzerland.

IACS STUDENTS TEACH HPC WORKSHOP AT POLAR 2018

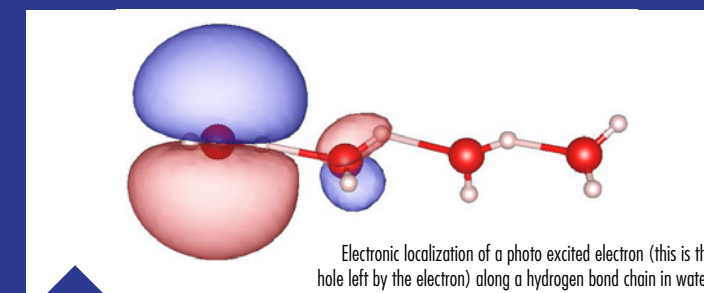
IACS graduate students Casey Youngflesh (caseyyoungflesh.com) and Catherine Foley (catherinefoley.weebly.com) from Associate Professor Heather Lynch's lab kicked off this year's POLAR 2018 conference by teaching a 2-day Software Carpentry/High Performance Computing workshop. The POLAR 2018 conference was held in Davos, Switzerland from June 15-26 and was made possible by an NSF Research Coordination Grant (polar.crc.nd.edu/), which endeavors to develop better cyberinfrastructure resources for complex analyses conducted by polar scientists.

GRANT HIGHLIGHTS



Adaptive Remapping for Multiphysics Coupling

Led by IACS core faculty member Xiangmin Jiao: Multiphysics coupling, such as global climate modeling, often requires transferring solutions at the interfaces of the coupled systems. Increasingly, higher order methods and higher resolution meshes are used by the physics models, the interface meshes between the physics models maybe non-matching, and the solutions to be transferred may be nonsmooth, involving large second derivatives or weak discontinuities. These properties require robust and efficient solution transfer methods. In this project Prof. Xiangmin Jiao and his students develop an adaptive solution transfer method, which takes advantages of both approaches. Their approach applies piecewise weighted least square fitting to obtain an intermediate approximation of the solution with high-order accuracy. It also applies a regularization process, which first identifies the nonsmooth regions and then uses a Petrov-Galerkin formulation to enforce local conservation in a weighted sense. This project is supported under the Scientific Discovery through Advanced Computing (SciDAC) program in the US Department of Energy Office of Science, Office of Advanced Scientific Computing Research with Los Alamos National Laboratory.



Electronic localization of a photo excited electron (this is the hole left by the electron) along a hydrogen bond chain in water.

Development and application of methods for understanding interfacial charge transfer in photocatalytic water splitting materials

Led by IACS core faculty member Marivi Fernandez-Serra: This proposal is focused on understanding the coupling between electronic and ionic degrees of freedom at the interface of materials with water for green energy applications like photocatalysis.

Certain photocatalytic reactions on semiconductor surfaces produce hydrogen and hence have the potential to address our growing energy needs. However, the possible reaction intermediates and trajectories associated with such photon-driven reactions are currently not well understood. This grant studies the response of molecular systems upon photoexcitation. The group is particularly interested in the evolution of a system on the excited-state potential energy surface, and the interaction of the molecular intermediates with its surroundings after excitation that further leads to a desired reaction. They use ab initio nonadiabatic simulations to study the time evolution of photoexcited states. Their choice is to simulate the coupled electron-ion dynamics using real-time Time Dependent Density Functional Theory (rt-TDDFT)-based Ehrenfest dynamics. This appears to be a promising nonadiabatic dynamics scheme given the considerable sizes of the molecular systems of interest. We compare the ultrafast dynamics of the "photogenerated-hole" as captured by rt-TDDFT Ehrenfest dynamics with the commonly used Born-Oppenheimer dynamics at similar time scales and identify the key physical characteristics that differentiate one from the other, thereby empirically testing a more computationally intensive nonadiabatic scheme for elucidating the physics of photoexcited systems. This project is supported by the US Department of Energy.

IACS Student Association

By IACS Student Association President Jonathan Rawski

The IACS Student Association continues its mission of providing IACS students and faculty with interesting, cross-disciplinary events and networking opportunities.

SOCIAL EVENTS

Some of the association's goals are to create social networking events for their members and also to attract new members to the institute. This year the association hosted a beginning-of-the-year social in the IACS seminar room, which was attended by a record 70+ participants. Additionally, the association continues to organize the Student Seminar Series, where IACS affiliated or core students present their work to an interdisciplinary audience in an informal setting with a catered lunch. This year the talks have been from a wide variety of disciplines: engineering, linguistics, and sociology to name a few. The upcoming semester promises to keep this going with seven

more talks planned for spring. The association precedes each student seminar with an informal practice talk for the speakers, where members give feedback on the presentation and organization of the talk as well as suggestions for presenting to a multidisciplinary audience. These pre-seminar sessions are helpful for presenters and allow the students in IACS to get to know one another as research colleagues. In the words of one presenter, "I would never have known how to talk across disciplines without this session. Thanks for the help!"

WORKSHOPS

In addition to social and student seminar events, the association organizes high-profile workshops. These workshops in beginning and more advanced programming languages are regularly held, through our Software Carpentry membership, along with opportunities for select IACS members to be trained as Software Carpentry instructors. The programming workshops are open to anyone at SBU and allow IACS to reach out to the university and show how programming and computational methods can be applied in any discipline.

INVITED SPEAKERS

Finally, the student organization invites noteworthy speakers, whose accomplishments cross the disciplinary boundaries of many IACS research areas, to visit with association students and to give a presentation. This year we are pleased to welcome Dr. Karl Friston, professor of neurobiology at University College London, who will give a Provost Lecture in April. Dr. Friston is a pioneer in medical imaging, theoretical neuroscience, and statistical inference, whose work has earned him numerous accolades and cemented him as one of the most well-known names in neuroscience.

The association's executive board consists of Aniello de Santo, Alena Aksenova, Jonathan Rawski, Aditi Ghai, and Joel Anderson. To learn more about the association, to view the calendar of events, or to join its ranks, you can visit <https://you.stonybrook.edu/iacssa/>.

Outgoing association president Aimilios Sofianopoulos talks to incoming students about future association events.



Graduate students Panu Sam-Ang from Applied Mathematics and Statistics and Connor Behan from Physics and Astronomy enjoy the free food at the association social.



Student Association Events

March 8, 2018

IACS Social Mixer: Cocktails & Conversation

April 25, 2018

Roy Shilkrot
IACS Brown Bag Lunch: Deep Human-Machine Integrated Learning for Assistive Computer Agents

September 12, 2018

Matthew Reuter
IACS Brown Bag Lunch: DOxygen

September 13, 2018

IACS Fall Student Social

September 19, 2018

Firat Coskun
IACS Brown Bag Lunch: Big Data

October 8, 2018

IACS Student Workshop: Advanced Python Programming

October 31, 2018

Aditi Ghai
IACS Brown Bag Lunch: How to Get an Internship at a National Laboratory

November 21, 2018

Rathish Das
IACS Brown Bag Lunch: Parallel Algorithms and Performance Modeling

Student Association Seminars

February 7, 2018

Martin Smyth, Stony Brook University Sociology
Rapid Information Flows and Emergent Political Phenomena: A Complex Systems Theoretic Approach

February 21, 2018

Gaurav Guleria, Stony Brook University Mechanical Engineering
Investigation of Reactivity Controlled

Compression Ignition (RCCI) Using 3D CFD Simulations

February 28, 2018

Junting Ye, Stony Brook University Computer Science
Nationality Classification Using Name Embeddings

April 11, 2018

Hossep Dolatian, Stony Brook University Linguistics
Reduplication with 2-Way Deterministic Finite-State Transducers

October 24, 2018

Sienna Thorgusen, Stony Brook University Sociology
Identifying Differences in Social Entrepreneurship and Corporate Social Responsibility Discourse Across Disciplines and Time

November 14, 2018

Jonathan Rawski, Stony Brook University Linguistics
Learning with Partially Ordered Representations



IACS NEWS



Members of our dynamic recruitment team at the 2018 Society for Advancement of Chicanos/Hispanics and Native Americans in Science (SACNAS) National Diversity in STEM Conference in San Antonio, TX (from left): Folnetti Alvarez (PhD Student, Molecular & Cellular Pharmacology); Adelle Molina (PhD Candidate & STRIDE Fellow, SoMAS); Dr. Isaac Carrico (Chemistry); Dr. Miguel Garcia-Diaz (Molecular & Cellular Pharmacology); Dr. Angel Gonzalez (Center for Inclusive Education); Vanessa Lynn (PhD Candidate, Sociology); and Yalile Surriel (PhD Candidate, History).

IACS RECRUITS!

In 2018, IACS broadened its recruitment efforts and visited six college campuses engaging approximately 150 prospective graduate students. Compared to fall 2017, IACS tripled the number of students reached through campus visits. Teams of IACS/STRIDE faculty and staff, led by Diversity Outreach Coordinator Rosalia Davi, traveled to Maryland, New Jersey, and the Long Island/NYC metro area where they met diverse students interested in pursuing graduate degrees in Computer Science, Electrical Engineering, Biology, Physics, Mathematics, and more.

In addition to on-campus visits, IACS also hosted its first virtual information session with Wofford College in South Carolina. In collaboration with Dr. Angela Shiflet and hosted by Dr. Beau M. Christ, Assistant Professor of Computer Science at Wofford, we presented to undergraduates in Dr. Christ's Modeling and Simulation course. IACS Professor Marivi Fernandez-Serra and graduate student Vidushi Sharma fielded questions about their work, the graduate experience at Stony Brook, as well as the application process.

IACS also returned to SACNAS - The National Diversity in STEM Conference in San Antonio, TX (October 11-13). IACS Student and STRIDE Fellow Adelle Molina (SoMAS) represented IACS and the NSF STRIDE program at this large-scale diversity conference, where the recruitment team connected with over 110 prospective students seeking graduate and summer research opportunities.

IACS also increased its efforts to engage external students studying for the summer at Stony Brook University. Students participating in SBU's Research Experience for Undergraduates Nanotechnology for Health, Energy and the Environment and the NIH IMSD-MERGE summer research programs learned about computational science and its many applications through presentations provided by IACS students and staff. On October 11, IACS also hosted its 2nd annual Information Session for any graduate student interested in learning more about the institute, which drew 40+ students from across the university.

Other outreach activities included meeting with visiting interns from the Air Force Research Laboratory in Rome, NY. (An extraordinary participant from this trip submitted her PhD application in Applied Mathematics and Statistics for Fall 2019 admission.) IACS participated for the third year in Graduate School Preview Day, an annual event hosted by the Center for Inclusive Education. IACS Administrative Director Lynn Allopenna spoke with attendees during the Networking Lunch, as well as hosted an information session with faculty and students after the event.

It was a productive year for recruitment, and we look forward to staying in touch with all of the amazing prospective students we met in 2018. Special thanks to IACS/STRIDE faculty members Mónica Bugallo, Alan Calder, Barbara Chapman, Marivi Fernandez-Serra, Matthew Reuter and Thomas Woodson - and IACS/STRIDE students Joshua Comden, Sebastian Dick, Lisa Herbert, Zahraa Krayem, Adelle Molina, and Vidushi Sharma - for all of your time and support of IACS' recruitment efforts this past year!

IACS NEWS

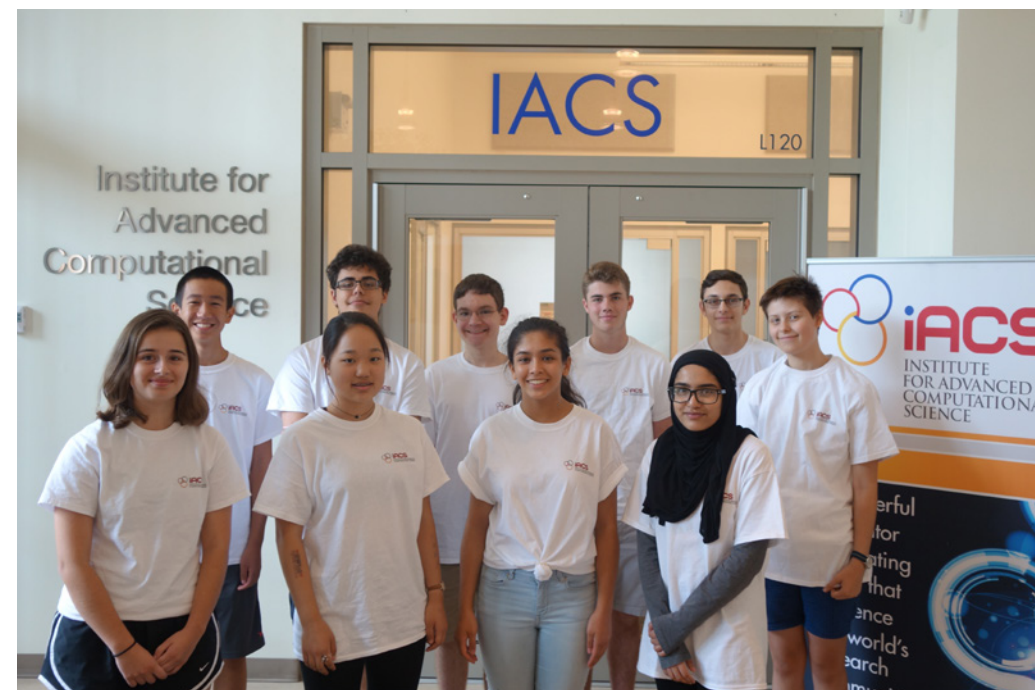
Community Outreach

NACLO

On January 14, IACS hosted a practice session for the North American Computational Linguistics Olympiad (NACLO). NACLO is a contest in which middle and high-school students solve linguistic puzzles using logic, reason, and computational principles. Fourteen middle and high-school students participated along with some of their parents and teachers, representing Dawnwood Middle School, Comsewogue High School, Half Hollow Hills High School East, Half Hollow Hills High School West, the Long Island School for the Gifted, and the Stony Brook School. Professor Christina Tortora (CUNY Linguistics) introduced the practice session with an overview of the science of language, and then the students broke into two groups to practice problems. The groups were mentored by five graduate students from the department of Linguistics. Stony Brook University Linguistics Professors Jeffrey Heinz, Richard Larson, and Lori Repetti were also in attendance. Professor Larson said, "I thought the intro presentation by Prof. Christina Tortora was terrific and engaging. And looking into the problem solving rooms afterwards, it was clear the kids were totally engaged. A great job and a fun afternoon!"



Middle and high school students and their parents from across Long Island gathered at IACS on Sunday, January 14 to practice for the upcoming NACLO contest. Photo by Prof. Jeffrey Heinz



IACS COMPUTES! HS SUMMER CAMP

For the past 4 years, IACS has offered IACS Computes!, a prestigious and highly-regarded two-week summer camp designed specifically for selected junior and senior high school students from the Tri-State area who express interest in learning computer programming skills and languages. Students have attended the camp from schools as far away as Brooklyn, Queens and Hillsborough, NJ as well as one visiting student from France.

With no assumed prior knowledge or experience, the curriculum introduces programming using the Python language and emphasizes development of algorithmic thinking and problem solving. From IACS faculty and graduate students, participants learn about using big-data analytics and high-performance computing to solve problems in science and engineering, and they participate in team projects motivated by these same research challenges. As in previous years, the 2018 student workshop proved to be another IACS success.

As we pull together our sixth annual retrospective report, we take a moment to stop pushing ahead and instead look back in review to appreciate the opportunities we've had to grow, excel, and propel the institute forward. None of the successes we have had or those that are yet to come would be possible without the generous support of our endowers and supporters, and for that we are very grateful and say thank you.

The accomplishments we are most proud of in 2018 are:

- Increased our awards to our IACS students with the highest total count yet: 8 Junior Researcher Awards; 9 Young Writer Awards, and 17 Travel Awards
- Completed our fourth annual IACS Computes! high-school summer camp with an equal number of male and female participants
- Continued to support a highly productive research environment through providing full and partial financial support for staff and student assistants
- Held 12 programming workshops, the most since inception
- Officially enrolled 30 graduate students, with another 15 in the pipeline, in the Certificate for Data and Computational Science and Engineering
- Widened our recruiting efforts to include schools in New Jersey and Maryland, and held our first virtual recruiting event with Wofford College in South Carolina
- Hosted 23 speakers in our faculty seminar series
- Hired Jessica Rojahn as our dedicated web and social media point of contact and Bradley Spitzbart as a Research Programmer
- Twenty-six percent of our annual operating budget went to supporting students either through direct payroll, awards, or travel reimbursement
- IACS core faculty published 40 papers, submitted 39 grants and won \$1.95M in external funding

Future goals are:

- Finish the recruiting and installation of our two endowed chair positions
- Continue to partner with university leadership to build a world-class computational infrastructure with technical support to free faculty and students to focus on creativity and innovation

Interested in investing in Stony Brook University?

Call 631-632-6330 or visit stonybrook.edu/foundation

JR. RESEARCHER AWARD

- Alena Aksenova, Linguistics – Graf
- Jonathan Rawski, Linguistics – Heinz
- Bhavya Ghai, Computer Science – Mueller
- Junting Ye, Computer Science – Skiena
- Bento Goncalves, Ecology & Evolution – Lynch
- Mikhail Ignatov, Applied Mathematics and Statistics – Kozakov
- Maria Guadalupe Barrios Sazo, Physics & Astronomy – Zingale
- Sebastian Dick, Physics & Astronomy – Fernandez-Serra

TRAVEL AWARD

- Md Abdullah Shahneous Bari, Computer Science – Chapman
- Shilpi Bhattacharyya, Computer Science – Chapman
- Mozghan Rahimi Boldaji, Mechanical Engineering – Mamalis
- Lequan Chi, SoMAS – Wolfe
- Aniello De Santo, Linguistics – Graf
- Hossep Dolation, Linguistics – Heinz
- Fan Wang, Computer Science – Shilkrot
- Catherine Foley, Ecology and Evolution – Lynch
- Prachi Gupta, Applied Mathematics and Statistics – Deng

- Changnian Han, Applied Mathematics and Statistics – Deng
- Rachael Herman, Ecology and Evolution – Lynch
- Abigail Hsu, Applied Mathematics and Statistics – Glimm
- Maureen Lynch, Ecology and Evolution – Lynch
- Jonathan Rawski, Linguistics – Heinz
- Michael Schrimpf, Ecology and Evolution – Lynch
- Aimilios Sofianopoulos, Mechanical Engineering – Mamalis
- Zeyang Ye, Applied Mathematics and Statistics – Deng

YOUNG WRITER'S AWARD

- Michael Schrimpf, Ecology and Evolution – Lynch
- Alexander Borowicz, Ecology and Evolution – Lynch
- Mikhail Ignatov, Applied Mathematics and Statistics – Kozakov
- Meghan Henderson, SoMAS – Nye
- Wenbo Wang, Materials Science and Chemical Engineering – Trelewicz
- W. Streit Cunningham, Materials Science and Chemical Engineering – Trelewicz
- Aditi Ghai, Applied Mathematics and Statistics – Jiao
- Mohammad Ruhul Amin, Computer Science – Skiena
- Saeed Boor Boor, Computer Science – Kaufman

Funding Agencies

MICHIGAN STATE
UNIVERSITY



LOS ALAMOS
National Security, LLC



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Alan Calder

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



Barbara Chapman

Barbara Chapman is 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 OpenMO directive-based programming standard since 2001. She also is an active participant in the OpenSHMEM and OpenACC programming standards efforts. Her work explores programming models for large-scale computing with a focus on node programming, strategies for runtime optimizations, compiler-tool interactions and high-level programming models for embedded systems.



Rezaul Chowdhury

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



Marivi Fernandez-Serra

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.



Robert Harrison

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



Jeffrey Heinz

Jeffrey Heinz is a Professor of Linguistics who conducts research in several related areas including theoretical and mathematical linguistics, theoretical computer science, computational learning theory, robotic planning and control, and artificial intelligence. In addition to dozens of publications in journals and peer-reviewed book chapters and conference proceedings, he has co-authored a book on grammatical inference for computational linguists, edited two books, and guest-edited special issues of the journals *Machine Learning* and *Phonology*.

He obtained his Ph.D. from UCLA in 2007 and spent ten years as a professor at the University of Delaware before coming to Stony Brook in 2017. The Linguistic Society of America recognized Heinz with its 2017 Early Career Award for his "contributions leading to a new computational science of inference and learning as applied to language."



Xiangmin Jiao

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



Marat Khairoutdinov

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 (rossby.msrc.sunysb.edu/~marat/SAM.html), 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.



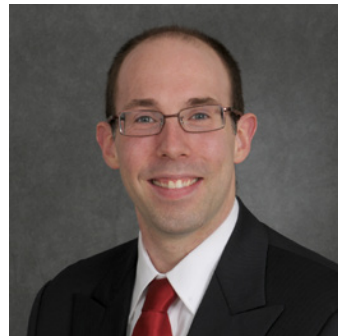
Predrag Krstic

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



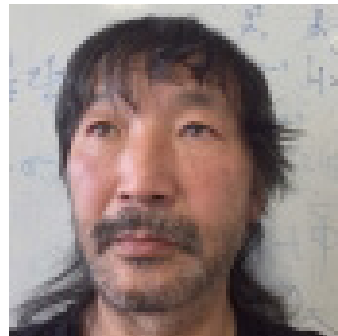
Heather Lynch

Heather J. Lynch is an Associate Professor of Ecology & Evolution at Stony Brook University and has just transitioned to become an IACS core faculty member. Prior to Stony Brook, Dr. Lynch was an Adjunct Professor of Applied Math and Statistics at UC Santa Cruz and a Research Scientist in the Biology Department at the University of Maryland. Dr. Lynch received her A.B. in Physics from Princeton University in 2000, an A.M. in Physics from Harvard University in 2004, and a Ph.D. in Organismal and Evolutionary Biology from Harvard University in 2006. Dr. Lynch's research is focused on spatial population dynamics of Antarctic penguins, with a particular focus on statistical and mathematical models to integrate patchy time series with remote sensing imagery. These data will allow Dr. Lynch and colleagues to develop mathematical models to explore how coloniality constrains the colonization and extinction of individual habitat patches and, ultimately, the metapopulation dynamics of colonial seabirds.



Matthew Reuter

Matt Reuter is an Assistant Professor in AMS. 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 more than 20 peer-reviewed journal articles. He was also the recipient of a U.S. DoE Computational Science Graduate Fellowship for most of his graduate studies at Northwestern.



Hideo Sekino

Hideo Sekino joined IACS as a part-time core faculty member in 2016. Prior to coming to IACS, he was a professor at the Toyohashi University of Technology in Japan. He received his PhD from Tokyo Institute of Technology in 1982. His research interests are in theoretical and quantum chemistry, computational science, simulation science, and computational science for temporal arts. He is a visiting professor in the Department of Physics at the Tokyo Institute of Technology, a major member of the Natural and Artificial Science Research Association <http://n-as.org/> and he runs 'Rakudoan', a performance art space in Tokyo <http://n-as.org/rakudoan/index.htm>.



Jason Trelewicz

Jason Trelewicz is an Associate Professor of Materials Science and Engineering at Stony Brook University with a joint appointment in the Department of Materials Science and Chemical Engineering and the Institute for Advanced Computational Science. His research explores the science of interface engineered alloys using in situ and analytical characterization tools coupled with large-scale atomistic simulations to design materials for extreme environment applications. Professor Trelewicz received his Ph.D. in Materials Science and Engineering from the Massachusetts Institute of Technology in 2008. Prior to joining the faculty at Stony Brook University, he spent four years as Research Director at MesoScribe Technologies, Inc. responsible for managing the development of harsh environment sensor technologies produced by additive manufacturing processes. Professor Trelewicz is a recipient of the 2017 DOE Early Career Award and 2016 NSF Faculty Early Career Development (CAREER) Award. He was also selected as the Inaugural Recipient of the Fusen and Yijen Chen Prize for Innovative Research in 2018, received the 2015 TMS Young Leader Professional Development Award, and was selected as a TMS representative for the 2014 Emerging Leaders Alliance Conference. Professor Trelewicz is an active member of the Materials Research Society (MRS), The Minerals, Metals, and Materials Society (TMS), and ASM International.



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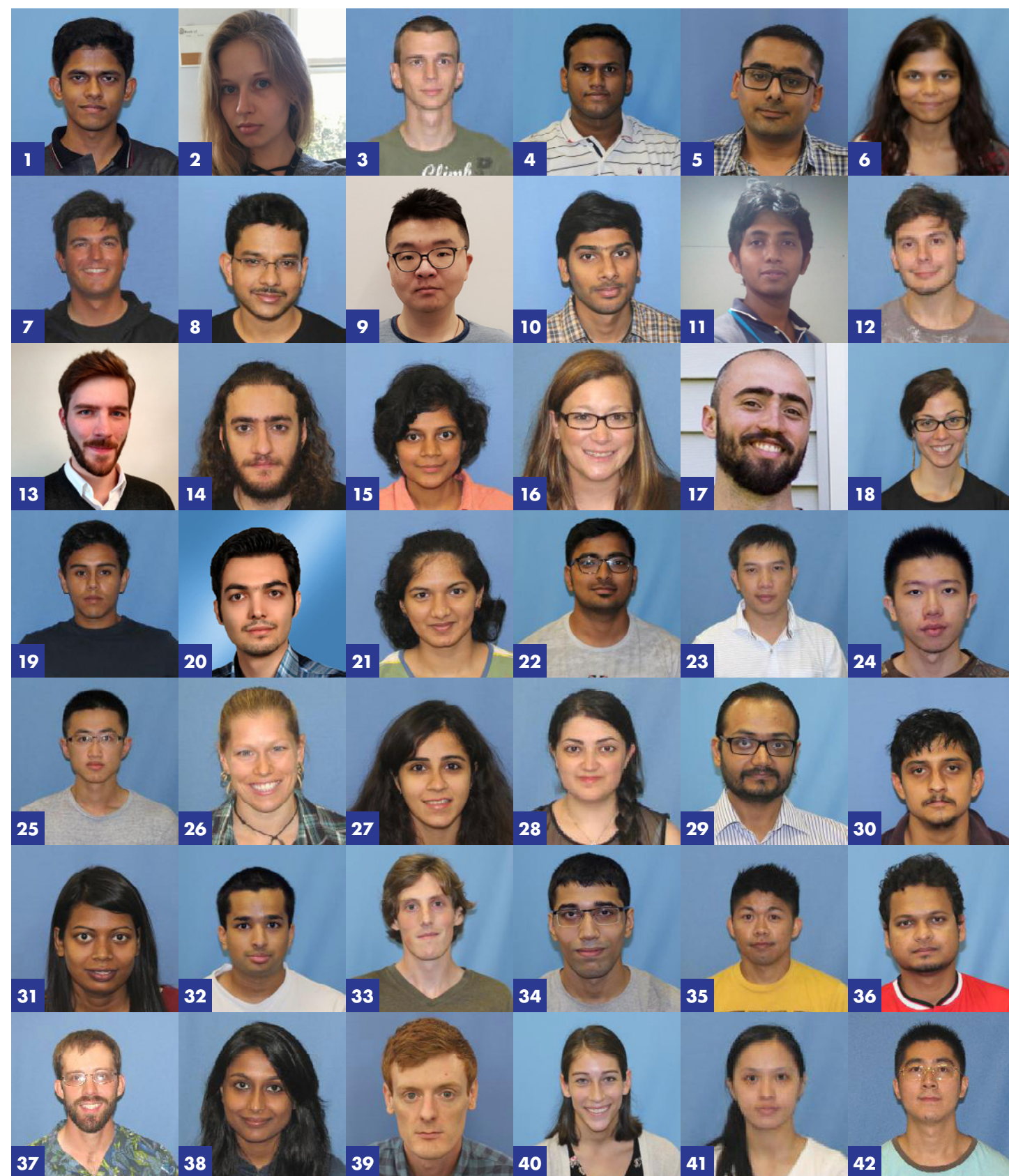
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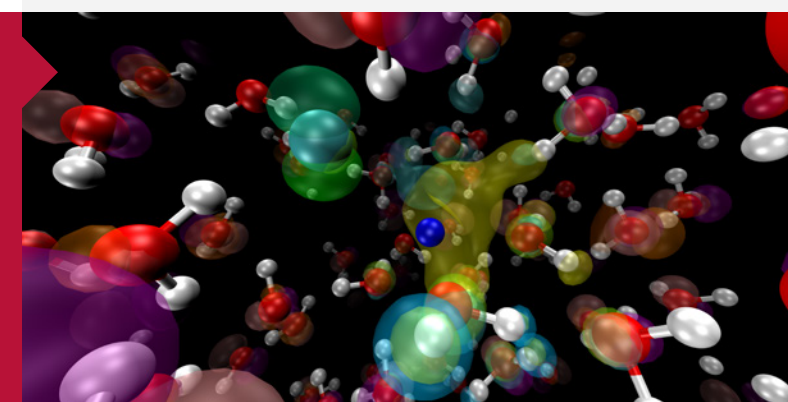
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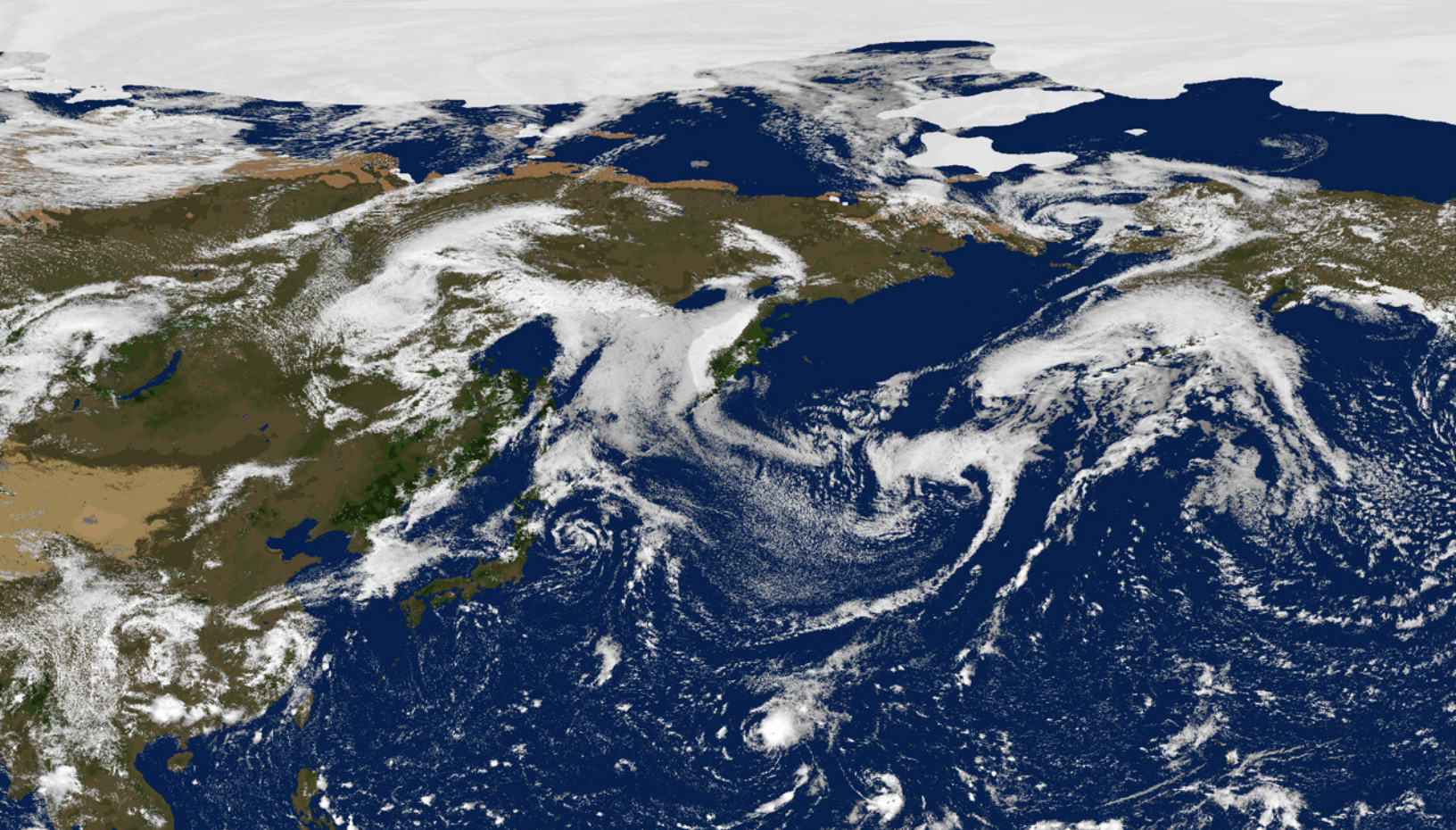


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Image by
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Ab initio simulation
of Na and Cl ions in
water, with the density
of the transferred
electron plotted.





Cover Image by Marat Khairoutdinov
Snapshot of the Earth as simulated by the System for Atmospheric Modeling using 4 km global grid resolution. The model uses more than 3 billion grid cells and runs 6 times faster than real time using 4608 compute cores on Cheyenne supercomputer at the National Center for Atmospheric Research.

