2017 ANNUAL REPORT

iACS
INSTITUTE FOR ADVANCED COMPUTATIONAL SCIENCE

These data represent simulated animals on a three-dimensional landscape, a project inspired by three-dimensional imagery of penguins nesting in the Antarctic as captured by un-manned aerial vehicles (UAVs).
Credit: Philip McDowall

MESSAGE FROM THE IACS LEADERSHIP TEAM

This year marks our 5th anniversary — the time has gone by so fast, and this past year has been just as exciting as those before. Our first external five-year review committee met simultaneously with our advisory board, and we are delighted to have received extremely positive feedback and many supportive suggestions; details follow later in the report.

It is a great joy to welcome new core faculty members Associate Professor Heather Lynch from Ecology & Evolution and Assistant Professor Jason Trelewicz from Materials Science & Chemical Engineering; both were previously affiliated and were so engaged and passionate about our mission that we sought their full inclusion. Heather develops and applies advanced data and statistical methods to conservation biology, for example applying machine learning and other techniques to process truly huge image data sets to create 3D maps of penguin and seal populations in the Antarctic. Jason is interested in high-strength and radiation-tolerant nanomaterials for extreme environment applications, and you will have read in previous reports about his successful leadership of the HPCny industry-outreach project at Stony Brook. Both Heather and Jason exemplify the IACS multidisciplinary approach to science by creatively fusing within their own groups experiment/observation with advanced computation.

We are also extremely fortunate to have found Dr. Jennifer McCauley who is our new Science Training & Research to Inform DEcisions (STRIDE) program coordinator. STRIDE is a five-year, $3M National Science Foundation Research Traineeship grant. Jennifer holds a PhD in industrial and organizational psychology, with experience as an administrator at the Albert Einstein College of Medicine and Memorial Sloan Kettering. Within less than a year, her leadership has helped moved the STRIDE program forward from concept to implementation, and, for example, we are thrilled to report the approval by the State Education Department of the program's 15-credit advanced graduate certificate. We have eight students formally registered in the certificate program with more poised to join in the coming semester. This year has seen the first cohort of grant-funded fellows; the first summer of STRIDE-related internships; a host of well-attended brown bag lunches; the first annual STRIDE-con; a new website; and several recruiting trips. The faculty involved along with the program coordinator have done a stellar job of steering the program into the future.

Some additional highlights in the remaining space: Our pursuit of external funding continued this year with 24 proposals submitted for a total of $20,652,518: three proposals are still pending (valued at $5,076,687) and 14 were awarded (valued at $2,806,268). This summer, IACS held our first Research Experience for Undergraduates entitled Data + Computing = Discovery with funding from multiple partners across campus. We received over 60 applications for 10 spots (four females, two underrepresented minorities), all of whom came from such diverse fields as astrophysics, biochemistry, computer science, biomedical engineering, physics, chemistry, and applied mathematics. All faculty were extremely impressed with the maturity and skills of the students who had a real impact on our research — we are anticipating multiple joint publications.

In addition to our gracious endowers and the SBU university leadership (especially the Provost and his team), this year we would like to give special thanks to Dr. Melissa Woo, the Senior Vice President for Information Technology and Chief Information Officer, who is actively leading the charge to establish campus-wide research computing and data, including making significant investments in staff, students (page 8) and infrastructure (including our new-world class 200-Gbit/s internet connection). We share her vision and sense of urgency. Finally, we should thank our tireless HPC system administration team (Firat Coskun and Eric Rosenberg) who successfully navigated significant technical and other hurdles to make a great success of the SeaWulf system that is now the core of the emerging computing infrastructure.

Robert Harrison
IACS Director

Alan Calder
IACS Deputy Director

Lynn Allopenna
IACS Administrative Director

OUR 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, multidisciplinary 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 faculty spanning chemistry, materials by design, condensed matter, astrophysics, atmospheric science, nanoscience, linguistics, ecology, applied mathematics, and computer science. Another approximate 40 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.

OUR 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.


Women In Science and Engineering (WISE) Honors program offers educational and professional science, technology, engineering, and mathematics (STEM) opportunities for undergraduate female students at the university by facilitating individual, institutional, and social change. This past year, two of our IACS PhD graduate students from Physics and Astronomy, Donald Willcox and Maria Barrios Sazo, taught a course for WISE undergraduates focusing on computational science in astrophysics; an introduction to basic computation. On March 28, the group visited the IACS computer clusters LI-red and Handy, which are housed on the second floor of the IACS building.

NEW HIRES
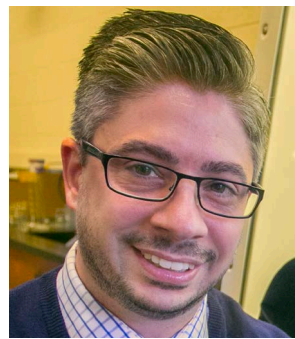
Jason Trelewicz

Jason Trelewicz is an Assistant Professor in the Department of Materials Science and Chemical Engineering at Stony Brook University and recently transitioned to become an IACS core faculty member. Prof. Trelewicz's research is on the science of interface engineered alloys with particular emphasis on high-strength and radiation-tolerant nanomaterials for extreme environment applications. His research group, the Engineered Metallic Nanostructures Laboratory, couples novel processing techniques and in situ characterization tools with large-scale atomistic simulations in the design of hierarchically structured metallic alloys. Materials including solute-stabilized nanocrystalline alloys, crystalline-amorphous nanolaminates, and metallic glass matrix composites are synthesized through electroforming, sputter and pulsed laser deposition, and additive manufacturing techniques, and used to build a new understanding of mechanisms responsible for thermal stability, mechanical behavior, and radiation damage. Prof. 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 in industry as a Principal Investigator at MesoScribe Technologies, Inc. responsible for managing technology development and transition on over a dozen DOD, DOE, and NASA research programs. Professor Trelewicz is a recipient of the 2017 DOE Early Career Award for "Enhancing the Performance of Plasma-facing Materials Through Solute-stabilized Nanostructured Tungsten Alloys" and the 2016 NSF Faculty Early Career Development (CAREER) Award for "Interface Engineered Amorphous Alloys for Thermoplastic Forming of Ductile Bulk Metallic Glasses".

IACS Core Faculty member Matthew Reuter, an Assistant Professor in the Applied Mathematics & Statistics Department (AMS), accepts an award for Excellence in Teaching from the College of Engineering and Applied Sciences (CEAS). Here he is pictured with IACS Director Robert Harrison (center) and CEAS Dean Fotis Sotiropoulos. Professor Reuter was nominated for the award by AMS Chair Joseph Mitchell after consultation with numerous graduate and undergraduate students mentored by Professor Reuter.

Jennifer McCauley

Jennifer McCauley joined IACS in February 2017 as the STRIDE Program Coordinator. She holds a BA in psychology from Manhattan College, an MS in Career Development from the College of New Rochelle, and a PhD in industrial and organizational psychology from Capella University. Jennifer's professional experiences include administrative leadership and human resources management within higher education settings, including the Albert Einstein College of Medicine of Yeshiva University and Memorial Sloan Kettering Cancer Center. Prior to her hire at SBU, Jennifer worked as an independent career consultant.
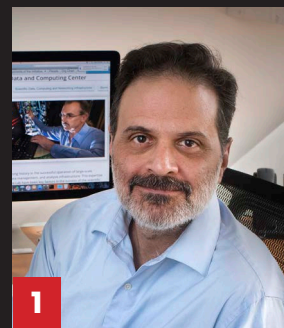
Heather Lynch

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.

NEW AFFILIATES

1. Francis Alexander
Deputy Director
Computational Science Initiative
Brookhaven National Laboratory

2. Adolfy Hoisie
Chair, Computing for National Security
Computational Science Initiative
Brookhaven National Laboratory

3. Meifeng Lin
Associate Computational Scientist
Computational Science Initiative
Brookhaven National Laboratory

4. Klaus Mueller
Professor
Computer Science
Stony Brook University

5. Robert Rizzo
Professor
Applied Mathematics and Statistics
Stony Brook University

6. Roy Shilkrot
Assistant Professor
Computer Science
Stony Brook University

7. Carlos Simmerling
Professor
Chemistry
Stony Brook University

8. Arnout van de Rijt
Professor
Sociology
Utrecht University

9. Krishna Veeramah
Assistant Professor
Ecology & Evolution
Stony Brook University

HEATHER LYNCH DEVELOPS NASA DATA CONTEST

Associate Professor Heather Lynch, an IACS faculty member, has developed a NASA-funded web tool, Mapping Application for Penguin Populations and Projected Dynamics (MAPPPD), to check on four species of Antarctic penguins. In order to work with the massive data set this program produces, Lynch and her former postdoc Grant Humphries came up with the idea of a data competition in the hopes that the winning model would allow her to expand MAPPPD's predictions. The full article can be read on nasa.gov entitled NASA-Funded Competition Reward Efforts to Predict Penguin Populations.

IACS SEMINAR SERIES

February 10, 2017
Fadi Abdeljawad, Sandia National Laboratories
Mescoscale Modeling of Grain Boundaries: From Segregation Phenomena to Faceting Instabilities

February 23, 2017
Michael Zingale, Stony Brook University
Computational Challenges of Modelling X-ray Bursts and Type Ia Supernova

March 2, 2017
Victoria Stodden, University of Illinois
Implementing Reproducible Computationally-enabled Research

March 9, 2017
Maria Klawe, Harvey Mudd College
Roundtable Discussion

March 21, 2017
Massimiliano Stengel, Materials Sciences Institute of Barcelona
Flexoelectricity From Density-Functional Perturbation Theory

March 29, 2017
Shantenu Jha, Rutgers University
Expeditions in Cyberinfrastructure for Scientific Applications

April 5, 2017
Brenda Rubenstein, Brown University
How to Make Compact Wave Functions on the Cheap: Stochastic Variational Algorithms for Quantum Physics and Chemistry

April 28, 2017
Martin McCullagh, Colorado State University
Developing Accurate Implicit Solvent Models for the Simulation of Hydrophobic Aggregation

September 14, 2017
Jeffrey Heinz, Stony Brook University
Subregular Complexity and Machine Learning

September 20, 2017
Stephan Irle, Oak Ridge National Laboratory
Some Problems of the Density-Functional Tight-binding Method for Chemical Applications and Possible Solutions

September 21, 2017
Lorena Barba, George Washington University
The Why and How of Reproducible Computational Research

September 28, 2017
Dr. Robert Kaita, Princeton Plasma Physics Laboratory
Challenges in Modelling of Plasma-Material Interactions for Fusion Applications

October 11, 2017
Jim Clark, Duke University
Uncertainty Quantification for NEON and Other Biodiversity Network Data with Hierarchical Bayes

October 12, 2017
Bill Fagan, University of Maryland
Perception and Memory in Animal Movement

November 2, 2017
Suresh Venkatasubramanian, University of Utah
Computational Philosophy and Data-driven Science

November 28, 2017
Steven Low, California Institute of Technology
Some Optimization Problems in Smart Grids

November 29, 2017
Kyle Gorman, Google
Minimally Supervised Text Normalization: Algorithms and Implementation

RESEARCH DAY

PROJECTS, PROGRAMS & EVENTS

NACLO - North American Computational Linguistics Olympiad at Stony Brook University
January 26, 2017

Music and Mathematics, Chaos or Chess
February 15, 2017 - composer Emily Howard, mathematician Lasse Rempe-Gillen & tuba virtuoso Jack Adler McKean

NVIDIA Workshops on Deep Learning, Pascal, CUDA and OpenACC
March 14 - 15, 2017

XSEDE HPC Workshop: MPI
April 18 – 19, 2017

IACS Research Day
April 26, 2017

Algorithms and Us
May 4-5, 2017

Data + Computing = Discovery – 8-Week Research Experience for Undergrads
June 12 - August 4, 2017

XSEDE Workshop: Scaling to Petascale
June 26 - 30, 2017

GPU Programming Workshop
June 26 - 28, 2017

NVIDIA Workshops on Deep Learning, Volta, CUDA & OpenACC
June 29 - 30, 2017

IACS Computes! HS Summer Camp
July 10 - 21, 2017

Polar HPC Workshop-Hackathon
August 1-4, 2017

2017 New York Scientific Data Summit (NYSDS) Data-Driven Discovery in Science and Industry
August 6 – 9, 2017 (New York University)

MEET THE NEW CROP
OF STUDENTS ON THE HPC SUPPORT TEAM

SBU undergrads and grads help cluster users maximize their time on SeaWulf

This year's group of students on SBU's HPC Support Team range from undergraduates to Master's to PhD students, all at the ready to help faculty and students navigate research roadmaps and technical issues when using SeaWulf, the 164-compute node system made possible by a National Science Foundation grant (#1531492).

The team members, led by Sr. HPC Engineer Firat Coskun, possess a broad breadth of academic backgrounds and have diverse interests and areas of expertise. This diversity is key to the team's success, as per Firat, "As our user community grows and encompasses more disciplines, especially those which recently started to reap the benefits of HPC, we've found the only way to provide the tailored level of support we strive for is by ensuring our pool of talent is just as diverse."

Austin Borger

Austin is a graduate student in computer science and has hosted several parallel computing workshops, both as a TA for XSEDE and as a presenter. In addition, he hosts office hours to provide live support for the HPC environment.

Dave Carlson

Dave Carlson is a third-year PhD student in ecology & evolution where he works on plant evolutionary genomics. At HPC support, Dave helps faculty and students from a variety of departments with bioinformatics analysis. In addition, he writes FAQ articles aimed at helping SeaWulf and LI-red users to successfully conduct their research in an HPC environment.

Ibironke Osipitan

Ibironke Osipitan is a junior studying computer science who is interested in the environmental sciences. She hopes to combine her computational skills with topics like computational physics and its uses for studying the properties of minerals and seismic hazard modeling.

Janet Vorobyeva

Janet Vorobyeva is a junior in computer science, minoring in electrical engineering. She has been improving usability of parallel computing software for the cluster and setting up tools such as Nvidia CUDA and OpenMP. She has also been working on the SeaWulf cluster to perform hardware upgrades and improve stability.

Jesse Talavera-Greenberg

Jesse Talavera-Greenberg is currently pursuing his Master's in computer science. On the HPC Support Team, he has been working on a subset of the NIST 800-171 compliance, Jupyter Hub/Notebooks, and providing technical support to the user community.

John Saputo

John is a senior in the Materials Science and Chemical Engineering Department working to improve the availability of SeaWulf's computational tools for solving problems in engineering and materials science. He is interested in using first principles calculations to predict the behavior of catalysts, and he conducts research in the Center for Thermal Spray working on developing materials for thermal management systems.

Ruhul Amin

Ruhul is a second-year PhD student in computer science, working on bioinformatics. On the HPC Support Team, he has been assisting the Sociology Department to leverage Deep Learning for Computational Social Science and has been developing local expertise in TensorFlow.

Ruiqi Rachel Wang

Ruiqi Rachel Wang is a third-semester graduate student in applied mathematics and statistics. She specializes in solving statistical computing problems with R but has also been assisting SeaWulf & LI-red users with general computational projects.

Ruyi Yu

Ruyi is a PhD student in Applied Mathematics and Statistics. He has been working with faculty from the School of Marine and Atmospheric Sciences on storm surge models.

Tyler Estro

Tyler Estro is a Master's student in computer science and a member of the File Systems and Storage Lab at SBU. His research interests include algorithms, machine learning and deep learning techniques, data science, and parallel computing. Recently, he has been collaborating with faculty in ecology & evolution on a project using SeaWulf to perform large-scale Web scraping and Tensorflow image classification to construct spatial and temporal distributions of seals in the Antarctic.

Support for these students 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.

HPC
CLUSTER USAGE

Number of SeaWulf users:
263

Number of departments represented by users:
30

Classes taught using SeaWulf:

AMS 530 Principles in Parallel Computing

AMS 536 Molecular Modeling of Biological Molecules

AMS 562 Introduction to Scientific Programming in C++

AMS 598 Big Data Analysis

AMS 487 Data + Computing = Discovery REU

BIO 303 Advanced Human Genetics

BS 3910 Introduction to Bioinformatics (taught at SUNY Old Westbury)

CSE 504 Compiler Design

CSE 590 Topics in Computer Science

CSE 628 Natural Language Processing

EST 508 Project in Global Operations Management

Assistant Professor of Computer Science Roy Shilkrot, left, and grad student and ethnomusicologist Jay Loomis collaborate on creating 3D replicas of ancient wind instruments.

3D COLLABORATIONS BUILD NEW WORLDS FOR MUSICIANS

In 2017, Stony Brook graduate student and ethnomusicologist Jay Loomis and assistant professor of computer science Roy Shilkrot teamed up to secure a grant to create 3D printed replicas of ancient wind instruments.

The goal? To give museum-goers an opportunity to interact with rare instruments rather than merely viewing them through a glass enclosure.

Loomis had been interested in wind instruments since he was a boy in Wisconsin, when he was struck deeply by flute music wafting from his car radio. After he moved to Long Island, his thirst for playing dovetailed with an insatiable curiosity about indigenous musical instruments. He hoped to build such instruments, as a way of sharing aspects of Native American culture with the public.

In his travels as an academic, he encountered musical virtuosos, acoustic experts and computer scientists who shared his passion. That passion gained momentum when Loomis became a teaching assistant at cDACT, the Stony Brook-based Consortium for Digital Art, Culture and Technology.

Through cDACT Director Margaret Schedel, Loomis connected first with Shilkrot and later Hideo Sekino, a visiting professor from Tokyo Institute of Technology, who is associated with the Institute for Advanced Computational Science at Stony Brook.

In spring 2017, Loomis and Shilkrot developed a 3D scanner and used desktop and professional 3D printers to recreate playable replicas of wind instruments, including flutes, ceramic ocarinas and whistles of different shapes and sizes. An integral part of the process was to recreate the sound of the original instrument and mirror its physical characteristics as well.

The greatest challenge the collaborators experienced was in designing the cavity of the instrument, which was essential to recreating the authentic sound. The results were encouraging but weren't as precise as Loomis wanted. Schedel recommended collaborating with Sekino due to his interest in the traditional Japanese flute known as a shakuhachi. After she introduced the two musicians, Loomis was inspired to feature the instrument in an electronic piece he co-composed with Timothy Vallier.

But it was Sekino's expertise with 3D printing that led Loomis to seek professor's advice on how to create a computer program to print ocarinas and other instruments.

Loomis was already able to approximate the sound by adjusting the distance between the holes on the ocarina. "I would fix some holes and print it again and, if I was lucky, it would be a three-step process of trial and error," said Loomis.

"But I was using a lot of plastic. It would be much easier if I was making them out of clay," he said. "I asked the professor why couldn't we look at the size of the holes and create a computer model to simulate the sound of the instrument all on computer, creating a 3D model based on computer models." Sekino said it would be difficult. But three months later he sent Loomis a video of one his friends playing a 3D shakuhachi. Sekino had shot an X-ray of the original instrument and translated that image using software data.

Now Sekino is on board with using 3D printing to create instruments that might otherwise be too labor-intensive to construct.

"His interests are twofold — as a scholar and as a performer," said Loomis. Loomis said that the bore, or shape of the inner surface of the tube, is perfectly cylindrical like a PVC pipe. Both Irish flutes and shakuhachis feature conical bores. "If you change the shape of the bore you change the sound of the flute," he said.

"The project lends itself to creating a bridge among science, music and engineering and the public," Loomis said.

Loomis added that there is a need to educate the public about indigenous musical instruments, which he does in schools, libraries, camps and for the past five years at Stony Brook University's Children's Defense Fund Freedom School.

"At the moment, the only musical instruments for sale in museums are generally children's toys," Loomis said.

For the moment, however both Loomis and Sekino are quite content to be fully engaged in the theory of building that better wind instrument and the big payoff — playing it in public.

THE FUTURE IS FUSION

The College of Engineering and Applied Sciences is proud to announce that Jason Trelewicz, PhD, has received the prestigious Early Career Research award from the U.S. Department of Energy's Office of Science. Professor Trelewicz will receive a total of $750K over five years to develop his project: "Enhancing the Performance of Plasma-facing Materials Through Solute-stabilized Nanostructured Tungsten Alloys."

The Department of Energy Early Career Research Program supports the development of individual research programs of outstanding scientists in their early careers. To be eligible, researchers must be untenured, tenure-track assistant or associate professors at a U.S. academic institution, and received a PhD within the last 10 years.

"The DOE Early Career award is among the most distinguished honors a faculty scientist can achieve," said Samuel L. Stanley Jr., MD, President of Stony Brook University. "Professor Trelewicz's work expands our research portfolio in clean energy technologies and advances Stony Brook's contributions for the emergence of fusion as an abundant source of carbon-free energy and embodies the big ideas that we apply to the STEM fields here at Stony Brook."

An assistant professor in the Department of Materials Science and Chemical Engineering in the College of Engineering and Applied Sciences, and director of the Engineered Metallic Nanostructures Laboratory, Professor Trelewicz is also an affiliate faculty member of the Institute for Advanced Computational Science, and director of the NYSTAR-funded High Performance Computing Consortium at Stony Brook University.

"We are exploring solutions to harness fusion as a sustainable energy technology, specifically addressing the grand challenge of developing state-of-the-art materials needed to build the reactor," Trelewicz said. He added that fusion would provide a safe, large-scale energy source that doesn't emit carbon dioxide or produce long-term radioactive waste.

Research topics are required to fall within one of the Office of Science's six major program offices: Advanced Scientific Computer Research, Biological and Environmental Research, Basic Energy Sciences, Fusion Energy Sciences, High Energy Physics, or Nuclear Physics. Awardees are selected from a national pool of university and national laboratory-based applications, based on peer review from outside scientific experts.

"We are very proud of Jason's extraordinary honor, as the DOE Early Career Award is testament to his marvelous professional trajectory," said Michael A. Bernstein, Provost and Senior Vice President for Academic Affairs at Stony Brook University. "We look forward to the critical contributions that Jason will make in sustainable energy research."

"Professor Trelewicz's break-through research into alternative energy embodies our core mission to develop sustainable, transformative solutions that are relevant to today's global challenges," said Fotis Sotiropoulos, Dean of the College of Engineering and Applied Sciences.

Professor Trelewicz received his Ph.D. in Materials Science and Engineering in 2008 from the Massachusetts Institute of Technology. Before joining Stony Brook in 2012, Trelewicz spent four years as Research Director at MesoScribe Technologies, Inc., where he managed technology development and transition with a focus on harsh environment sensors produced by additive manufacturing processes. Today, his research focuses on the design, synthesis, stability, and performance of interface engineered alloys through coupled simulations and experiments. Trelewicz is a recipient of the 2016 NSF Career Award and the 2015 TMS Young Leader Professional Development Award.

Project team pictured above. Back row L-R: Wenbin Lu, Anthony Curtis. Front row L-R: Barbara Chapman, and Abdullah Shahneous Bari Sayket. Delafrouz Mirfendereski is also a team member but was unavailable for the photo.
- Photo by Siobhan Becker

STRENGTHENING APPLICATION RESILIENCE:
PROFESSOR BARBARA CHAPMAN WINS NSF SPX AWARD

Written by Joseph Wolkin, Reprinted with permission from the Computer Science Department

Significant research in the area of computational power and large-scale application efficiency is being conducted by Professor Barbara Chapman, one of the latest computer science faculty members to receive an NSF funding award. Chapman has won the NSF Scalable Parallelism in the Extreme, otherwise known as an SPX award, for her research entitled, Cross-layer Application-Aware Resilience at Extreme Scale (CAARES).

The funded research is described as addressing the "challenges imposed by future extreme-scale architectures that will require dynamic programming approaches, where different software layers, potentially developed using different programming paradigms, will have to closely interact with each other."

"I'm extremely excited to represent Stony Brook University by winning this award thanks to the NSF," Chapman said. "The SPX award is one of the most prestigious in the industry, and it means the world to me to be named a recipient."

Chapman's work quantifies from a theoretical standpoint what the possible benefits are of gathering two well-understood resilience mechanisms, along with ABFT numerical libraries, in one representative application. Never proposed before, the target application is representative of computational science domains.

"In this project we will explore an in-staging data management runtime that combines multiple strategies using them appropriately at execution time based on data locality and/or importance," the proposal states. "For example, spatial/temporal data locality and user provided hints can be used to classify data based on its access pattern and access mode (read only, write only, or both), and this classification can be used to select appropriate data resilience strategies based on desired cost-benefit ratios."

The three-year project received over $300k in funding and will conclude in July 2020. In total, three graduate students will be hired to participate in the SPX project and they will work with the project lead, Anthony Curtis.

A faculty member at Stony Brook University since 2015, Chapman is a core part of the Institute for Advanced Computational Science and the Department of Computer Science. Additionally, she is a professor in the Department of Applied Mathematics and Statistics (AMS).

Prior to joining Stony Brook's College of Engineering and Applied Sciences, she served as the director of the Center for Advanced Computing and Data Systems (CACDS) at the University of Houston. While working in Houston, her research group 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.

Chapman also leads the Exascale Programming Models Laboratory, which aims "to increase programmer productivity, enhance application performance, develop novel implementation technologies that anticipate architectural changes and emerging user needs, and provide reference implementations of our ideas."

IACS JR. RESEARCHER AWARDS RUN THE GAMUT IN 2017

SIX STUDENTS FROM FIVE DIFFERENT DEPARTMENTS ARE THIS YEAR'S WINNERS

With an ever-increasing pool of stellar talent to choose from, the IACS Jr. Researcher Award committee found it the most difficult year yet to pick winners from the 19 candidates who applied for the prestigious award. "Each year this selection process is simultaneously both one of the most fun things we do and one of the toughest. Fun because we get to see lots of different disciplines through the fresh eyes of these talented young scientists, but also tough because we do have to make a selection. This year it was especially hard due to the large number of great proposals," said IACS Director Robert Harrison.

Of the 19 candidates, nine were chosen to move to the second round of the selection process which entailed giving a 12-minute research presentation to the awards committee followed by a few minutes of Q&A.

Two of the students, Aditi Ghai and Zeyang Ye both from Applied Math & Statistics, are returning award winners. The other four are new and come from such diverse backgrounds as Linguistics, Ecology & Evolution, Physics, and Computer Science. All, however, have a common theme: computational science is a strong component of their work. Other areas on which the candidates are judged: clearly communicating their goals and accomplishments; being knowledgeable and enthusiastic about their research; indicating innovation beyond their advisor's research; and imparting the significance and originality of their work.


Aditi Ghai (AMS) – Towards More Efficient and Robust Multigrid Methods

Originally from the northern part of India, Aditi has always been interested in knowing what goes on behind the scenes in life. Hoping to graduate within two years, she wants to get a job in industry or with a national lab doing research applications of numerical analysis and linear algebra.

Alena Aksenova (LIN) – Subregular Toolkit Implemented in Python

Alena is from Moscow, Russia. She has always been curious in general, and her love for math and languages brought her to linguistics. According to Alena, "I still haven't decided who I want to be when I grow up," but she wants to look for something that combines linguistics with industry and will allow robots to speak to humans.
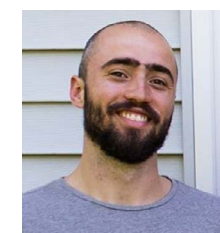
Bento Gonçalves (E&E) – Autonomous pan-Antarctic Pack-ice Seal Census using Remote Sensing and Deep Learning

Bento Gonçalves is originally from Bage, Brazil. When he came to SBU he was meant to work on theoretical ecology with a faculty member who unexpectedly retired, which left him looking for another advisor. He found Professor Heather Lynch and started working on applied ecology in the Antarctic. When he finishes his PhD he will either pursue a research position in industry with AI or return to Brazil to pursue a faculty position.

Maria Barrios Sazo (PHY) – Simulations of Black Widow Pulsars and White Dwarf Mergers using Castro

Originally from Guatemala, Maria enjoys math and algorithms and also some chemistry, so her research involves a lot of the areas that are interesting to her, plus, "Stars are very cool." After graduation, she would like to continue her research in industry creating simulations that involve high-performance computing.

Rathish Das (CS) – Auto-generating High Performing Implementations from Problem's High Level Description

Rathish hails from Calcutta, and as a young boy he was greatly influenced by his physics teacher who fueled his interest in science and math. His research involves theoretical and practical aspects of high performing parallel computation. After graduation, he would like to remain in academia and will pursue a faculty position at a university.

Zeyang Ye (AMS) – Parallel Markov Chain Monte Carlo Methods for Optimization

Curiosity initially drew Zeyang to science. He writes parallel code and also redesigns parallel algorithms for the Markov chain Monte Carlo methods. After graduation, he plans to continue his research in industry. He wants to apply the parallel Markov Chain Monte Carlo methods to solving different problems in an extraordinary small amount of time.

STRIDE MARCHES FORWARD AFTER A HIGHLY PRODUCTIVE YEAR

Back row: STRIDE senior personnel Thomas Woodson, co-PI Christine O'Connell and program coordinator Jennifer McCauley. Front row: co-PIs Liliana Davalos and Heather Lynch

In September of 2016 IACS was awarded a $3M National Science Foundation Research Training grant, and this first year has seen multiple achievements and landmark accomplishments that are quickly moving the grant forward in meeting its program goals.

STRIDE (Science Training and Research to Inform DEcisions) provides science, technology, engineering, and math (STEM) graduate students with the necessary skills to translate complex data-enabled research into informed decisions and sound policies. The program combines students' science disciplines with advanced data visualization training along with effective science communication skills through courses offered at the Alan Alda Center for Communicating Science.

Some of the Year One highlights are:

- Approval of STRIDE's 15-credit advanced graduate certificate

- Eight students have officially registered for the certificate and have begun taking classes

- Faculty and students participated in a STRIDE-run mentoring training workshop

- This workshop prepared faculty and students for the STRIDE 3-mentor model; a student's advisor, an outside faculty mentor, and a more senior peer mentor from a previous cohort all work together to mentor a single STRIDE trainee

- Five trainees participated in summer internships

- Students interned at Brookhaven National Laboratory, Antarctic & Southern Ocean Coalition (ASOC), and the National Oceanic and Atmospheric Administration with all associated costs covered by the grant

- Six domestic trainees were awarded STRIDE fellowships

- Fellowships provide competitive stipends at NSF rates plus medical coverage, tuition, an allowance for books, and all fees covered by the grant

- Multiple Brown Bag lunches were held and well attended

- Topics ranged from the political and social aspects of science to more technical training, such as how to use the high-performance computer clusters

- Recruiting/educational trips were made to Sachem School District; SUNY at Purchase; and Adelphi University with more planned for the spring semester to Queens College, CUNY; College of New Rochelle; and the University of Maryland, Baltimore

- Annual events such as STRIDE-Con and Many Paths to Science drew in many students and faculty members to network and engage in science communication

STRIDE VISUALIZES SUCCESS

At the first annual STRIDE-Con event held in August, students and faculty were immersed in a day-long program featuring prominent speakers in communications, policy, and data visualization. The day kicked off with a talk entitled Talking Science: Putting Yourself Back in Your Science led by Dr. Christine O'Connell, Assistant Professor of Communicating Science. Drs. Larry Swanson and Kevin Reed, from the School of Marine and Atmospheric Sciences, led two engaging talks on marine policy.

After lunch, it was standing room only at the Wang Center as students and faculty piled in to hear the keynote speaker, Mr. Scott Berinato of the Harvard Business Review, discuss the importance of effective visualizations. Promoting his book Good Charts, Mr. Berinato demonstrated how to make visually compelling charts and graphs to best convey one's research.

Immediately following the keynote address, STRIDE held its first annual visualization contest. Mr. Berinato was on hand to share his expert advice and opinions on each of the visualization entries. Xin Zhou (School of Marine and Atmospheric Sciences) and Catherine Foley (Ecology & Evolution) were the award winners. The prize for winning the visualization contest was an all-expense-paid trip to Boston to attend the Edward Tufte visualization workshop.

IN THE COMMUNITY

On April 6, 2017, STRIDE was invited to partipate in a Sachem School District science fair.

(L-R) STRIDE students Emily Markowitz and Adelle Molina, along with STRIDE program coordinator Jennifer McCauley, presented their research to children and families and had an opportunity to practice communicating science to a lay audience.

IACS' FIRST RESEARCH EXPERIENCE FOR UNDERGRADS IS A RESOUNDING SUCCESS

Isabel Siergiej kayaks down the Nissequogue River.

Although the work undertaken by the students was a serious endeavor, not all elements of the program were strictly research. Students ventured down the Nissequogue River in kayaks, donned their alley shoes for a night at Port Jeff Bowl, and dined out as a group in Port Jeff Village. Other events that were part of the program were organized to help the students sharpen their soft skills, such as the Distilling Your Message workshop where Professor Christine O'Connell from SBU's Alan Alda Center for Communicating Science taught students the importance of communicating their science in layman's terms.

In March, a team of seven from SBU traveled to Puerto Rico to visit four campuses: Universidad Metropolitana (UMET), University of Puerto Rico School of Medicine, Medical Sciences Campus (UPR SOM), University of Puerto Rico – Cayey (UPR-Cayey), and University of Puerto Rico – Mayaguez (UPR-Mayaguez). School of Marine and Atmospheric Sciences PhD Graduate Student Adelle Molina, a Puerto Rican native, was our IACS student ambassador representing both IACS and the STRIDE Project (see page 14).

Adelle traveled with staff, faculty, students, and postdocs from SBU's Center for Inclusive Education (CIE) and met with more than 70 undergraduate and graduate students interested in summer research and graduate and postdoctoral training opportunities here on campus. Presentations were delivered in both English and Spanish to accommodate bilingual audiences. As a result of this trip, four candidates applied to the 2017 IACS Data + Computing = Discovery pilot summer research program, one of whom participated (Jonathan Vazquez, mentored by Research Professor Predrag Krstic).

Nine undergraduate students from across the country spent eight weeks at the Institute for Advanced Computational Science at SBU performing computational research. Here they accept their certificates of completion at the Research Symposium held on August 4 at the Wang Center. Pictured (L-R) Colin Bunner from University of Minnesota; Emily Gentles from University of Arkansas; Andreas Lietzau from SBU; Sofya Pugach from SBU; Yakov Pichkar from SBU; Desmond Shangase from SBU; Carlyn Augustine from University of Alabama; Isabel Siergiej from Cornell University; Jonathan Vazquez from Universidad Metropolitana; and Robert Harrison, IACS Director. Photo by Constance Brukin Photography

Students enjoy dinner together in downtown Port Jefferson.

From left: Professor Thomas MacCarthy, Karian Wright, and Adelle Molina in Mayaguez, Puerto Rico. (Photo Credit: Karian Wright)

The Institute for Advanced Computational Science (IACS) held its first Research Experience for Undergraduates (REU) this summer, and by all accounts the program was a huge success. "It has been a total joy and privilege to have these talented young scientists here," said IACS Director Robert Harrison. "They brought a vibrancy and energy that reminded us all of why we entered science in the first place."

The nine undergraduates from across the country began the 8-week Data + Computing = Discovery (DCD) program on June 12 and ended by presenting their posters at the Research Symposium held at the Wang Center on August 4. The symposium was the culmination of all REU programs on campus and was attended by over 100 people. Students stood next to the posters they created that detailed the results of their research and explained those results to the many onlookers who

stopped by. "I definitely would not have had this opportunity in Arkansas!" said DCD undergraduate Emily Gentles.

The students started the program by taking a week-long, IACS-sponsored Python course so they could be well-versed in the programming language most commonly used by their faculty mentors. The faculty involved work in a wide variety of scientific fields from Ecology & Evolution to Physics to Neurobiology, and the projects assigned to the students varied from simulating thermonuclear supernovae to analyzing neural activity datasets from mice to formulating algorithms applicable to quantum chemistry. "I like to interact with computers and algorithms to make science," said DCD student Jonathan Vazquez from Puerto Rico. "I'm working with Professor Predrag Krstic on quantum chemistry; I never thought I would be working on this topic, but it's really interesting."

Financing of the program was a team effort: Funds were received from the Office of the Vice President for Research, the College of Engineering and Applied Sciences, the Provost's Office, IACS, and through supplemental funding requests to the National Science Foundation (NSF)-sponsored grants AST-1211563 White Dwarf Mergers as Progenitors of Type Ia Supernovae and TESSE #1450344. Efforts are underway to submit a new proposal to NSF for funds to bootstrap future REU programs to be held at the Institute for Advanced Computational Science starting next summer.

In the fall, IACS participated in two of the largest conferences supporting underrepresented minority students in STEM: Richard Tapia Celebration of Diversity in Computing (Sept 20-23, Atlanta, GA) and SACNAS – The National Diversity in STEM Conference (Oct 19-21, Salt Lake City, UT). Participation in these national conferences increased the visibility of Stony Brook University and highlighted the unique resources available to traditionally underrepresented students pursuing graduate degrees in STEM that are offered through CIE and IACS.

STUDENT ASSOCIATION LOOKS AHEAD

Photo: (L-R) Outgoing President and founding member Aimilios Sofianopoulos, outgoing Vice President and founding member Mahdi Javanmard, incoming members Aditi Ghai as treasurer, Jonathan Rawski as president, Aniello De Santo as Communications Specialist; and Alena Aksenova as Vice President.

New faces and new ideas are on the horizon for the IACS Student Association. Outgoing President Aimilios Sofianopoulos is in the final stretch for his PhD dissertation and therefore has tapped Linguistics PhD student Jonathan Rawski to step into the role for next year. Aimilios has been largely responsible for organizing the majority of social events hosted by the association as well as inviting, organizing, and hosting several prestigious visitors, e.g. Jack Dongarra, from the University of Tennessee, and James Demmel, from the University of California Berkeley. "Having Professor Dongarra and Professor Demmel on campus was a great experience. Apart from their lectures that covered brilliant material and attracted a wide audience, we had the chance to meet them as people and discuss new horizons and the latest trends in computational science," said Sofianopoulos.

Although Aimilios will be sorely missed in his position as president of the association, Jonathan takes the helm early in the spring of 2018 and plans to hit the ground running with some new ideas for events and a plan to reinvigorate the association. "Joining IACS has been quite a pleasure. I welcome the opportunity to serve as president and to work to bring together students from across SBU. We have some wonderful new ideas already, and I will be working hard to bring them to fruition in the coming semester and year," said Rawski.

Some of the ideas the committee hopes to 'ring in' with the new year are:

- Changing the format for the IACS Student Seminar Series to a more informal, roundtable discussion

- Advertising the association's availability to have 'practice seminars' for slated student speakers

- Starting a brown bag lunch series on a myriad of topics related to computational science

- Reaching out to more students on a personal level to encourage them to participate in events as well as in association monthly meetings

- Ramping up the association's website and social media sites

Three more new faces on the executive committee are Alena Aksenova and Aniello De Santo, both PhD students in the Linguistics Department, and Aditi Ghai, a PhD candidate from Applied Mathematics & Statistics. Alena will take the place of Mahdi Javanmard as Vice President; Aditi will become treasurer; and Aniello will be in charge of web design and social media. Original member Joel Anderson has graciously agreed to carry on as the association's Secretary.

If you are interested in joining the IACS Student Association, send an email to:

Joel.S.Anderson@stonybrook.edu.

For more information about the association, you can visit:

https://you.stonybrook.edu/iacssa/.

Student Association Seminar Series

February 15, 2017
Mozhgan Rahimi Boldaji, Mechanical Engineering
Computational Fluid Dynamics Simulation of the Effects of Direct Water Injection on Advanced Combustion

February 22, 2017
Haochen Chen, Computer Science
The Hierarchical Paradigm for Graph Embedding

March 22, 2017
Prachi Gupta, Applied Mathematics & Statistics
A Parallel Computing Platform for Multiscale Modelling of Platelets

April 12, 2017
Jean Paul Nery, Physics & Astronomy
Temperature-Dependence of the Forbidden (222) Reflection in Silicon

May 3, 2017
Lukasz Orlowski, Applied Mathematics & Statistics
Interconnect Topology Discovery by Computational Cluster Emulation

May 16, 2017
Javier Dominguez, IACS
Deuterium Retention and Sputtering Processes of Boronized, Lithiated, and Oxidated Carbon Surfaces Facing Low-Temperature Fusion Plasma

September 27, 2017
Yang Zhang, Materials Science and Chemical Engineering
The Role of Grain Boundaries in Self-Atom Collision Cascade

October 25, 2017
Simon Divilov, Physics & Astronomy
Computational Experiments Meet Real Experiments: Finding the Right Answer Through Cross Validation

November 1, 2017
Longtao Han, Materials Science and Chemical Engineering
Synthesis of Boron-Nitride Nanomaterials in Plasma Volume

November 15, 2017
Donald Willcox, Physics & Astronomy
Stellar Explosion Mechanics: Properties and Physical Processes in White Dwarf Interiors

Student Association Events

April 6, 2017
IACS Networking Happy Hour, The Bench

April 20, 2017
Kathleen Knobe, Rice University
CnC: A Dependence Programming Language

September 7, 2017
Student Faculty Dinner, Fifth Season

October 12, 2017
Student Appreciation Night, The Bench

November 3, 2017
Google PhD Summit
New York City

November 8, 2017
James Demmel, University of California Berkeley
Communication-Avoiding Algorithms for Linear Algebra and Beyond

IACS' FIRST FIVE-YEAR REVIEW

IACS held its first 5-year review this past September, a 2-day event that featured student and faculty presentations, a poster session, a networking dinner, a student/board member lunch, and individual one-on-one 'speed meetings'. In addition to our regular Advisory Board members, the Provost invited four External Reviewers to attend as well, and two separate reports were written evaluating the institute and its accomplishments over the last five years.

The Meeting

A recommendation from the Advisory Board from the past year was to have more interaction with IACS students. As a result, we incorporated five student presentations from IACS Jr. Researcher Award winners, a student-only lunch with board members (attended by 25 IACS core and affiliate students), and a poster session with 16 research placards on display.

In addition to our eight faculty presentations and overall summary presentation by the director, we arranged speed meetings, in the same vein as speed dating, where individual committee and board members met with faculty behind closed doors, rotating to a new office every 30 minutes in four sessions. We wanted to ensure, both for students and faculty, that everyone had a chance to speak freely with committee and board members regarding their experiences at the institute.

The Report

The External Reviewers as well as the Advisory Board were pleased with the progress IACS has made, and, not surprisingly, there were many common elements in both reports.

The report from the Advisory Board noted significant accomplishments, including the growing body of publications by IACS faculty and researchers, the quality of the presentations by students and faculty, and the steady increase in research grant submissions and funding. The report also noted IACS' efforts in education, particularly the graduate Certificate in Data and Computational Science, and IACS' service to the University in acquiring, installing, and maintaining campus computational facilities. The section describing accomplishments concluded:

"To summarize, the programs of the institute are holistic, not focused only on research. They have created community among different disciplinary constituents of the University and they are augmenting the curriculum of the University in ways that respond to growing opportunities for large-scale simulation and large-scale data analytics."

> " For more than 20 years there has been widespread recognition of the great benefits of multidisciplinary research. However, despite good intentions, it has been extremely difficult to create organizational structures in which multidisciplinarity is an integral part of the culture. IACS is one of the very few institutions that have succeeded in the challenging goal of supporting top-quality research that achieves excellence both within and beyond disciplinary boundaries. "
>
> IACS Advisory Board member Margaret Wright, - Professor NYU

The report from the External Reviewers was similarly positive. Members were pleased with our progress and in agreement with (ongoing) recommendations of the Advisory Board. The report began by commending IACS Director Robert Harrison on the rapid development of IACS and, similarly to the Advisory Board, commended the publications and external funding of IACS faculty and researchers. The External Reviewers also noted that IACS plans for hiring are proceeding albeit not at the desired pace. The report from the External Reviewers also stressed an important point - IACS is most fortunate to have its generous endowment, the income from which helps provide support and provides a safe harbor in the often-stormy sea of funding.

Recommendations

Recommendations from the review include:

- IACS finding a way to brand itself, that is, to distinguish itself from other computational science centers. An external facing brand would reach a community well beyond the University and influence hiring and interest of students, and the Reviewers and Board suggested IACS embark on establishing a small number of areas of research focus common to IACS members. Specific suggestions for branding and image recognition, include:

  - maintaining open source software packages

  - leading week-long programs, e.g. ICERN at Brown University, and

  - competing for major prizes such as the Gordon Bell Prize

- IACS continuing to expand its academic efforts, including exploring revenue-generating opportunities

- IACS continuing its present recruiting campaign, particularly in filling the Endowed Chair positions

EXTERNAL REVIEWERS

1. Dr. Jeffrey Durachta
Engineering Lead for Software Development
Geophysical Fluid Dynamics Laboratory

2. Professor Leslie Greengard
Mathematics and Computer Science
New York University

3. Dean Brent Lindquist
College of Arts and Sciences
Texas Tech University

4. Dr. Bobby Sumpter
Deputy Director
Center for Nanophase Materials Sciences
Oak Ridge National Laboratory

ADVISORY BOARD MEMBERS

5. Professor Alan Aspuru-Guzik
Chemistry and Chemical Biology
Harvard University

6. Professor Mary Hall
School of Computing
University of Utah

7. Professor David Keyes
Director, Extreme Computing Research Center
King Abdullah University of Science and Technology

8. Dr. Lois McInnes
Senior Computational Scientist
Mathematics and Computer Science Division
Argonne National Laboratory

9. Dr. Wolfgang Wander
Technical Staff
Renaissance Technologies LLC

10. Professor Margaret Wright
Computer Science
New York University

AWARDS

JR. RESEARCHER AWARD

Alena Aksenova, Linguistics – Graf

Rathish Das, Computer Science – Chowdhury

Aditi Ghai, Applied Mathematics & Statistics – Jiao

Bento Goncalves, Ecology & Evolution – Lynch

Maria Guadalupe Barrios Sazo, Physics & Astronomy - Zingale

Zeyang Ye, Applied Mathematics & Statistics - Deng

TRAVEL AWARD

Md Abdullah Shahneous Bari, Computer Science – Chapman

Mozghan Rahimi Boldaji, Mechanical Engineering – Mamalis

Longtao Han, Materials Science & Chemical Engineering – Krstic

Cecilia O'Leary, School of Marine & Atmospheric Sciences – Nye

Aimilios Sofianopolous, Mechanical Engineering – Mamalis

Donald Willcox, Physics & Astronomy – Zingale

Delafrouz Mirfendereski, Computer Science – Chapman

Mahdi Javanmard, Computer Science – Harrison

YOUNG WRITER'S AWARD

Mozghan Rahimi Boldaji, Mechanical Engineering – Mamalis

Longtao Han, Materials Science & Chemical Engineering – Krstic

Maureen Lynch, Ecology & Evolution – Lynch

Philip McDowall, Ecology & Evolution – Lynch

Casey Youngflesh, Ecology & Evolution – Lynch

Yang Zhang, Materials Science & Chemical Engineering – Trelewicz

FUNDING AGENCIES

U.S. DEPARTMENT OF ENERGY

PRAIRIE VIEW A&M UNIVERSITY

Rensselaer

NASA Goddard SPACE FLIGHT CENTER

PRINCETON UNIVERSITY

LOS ALAMOS National Security, LLC

EDC NEW YORK STATE Economic Development Council

VIRGINIA POLYTECHNIC INSTITUTE AND STATE UNIVERSITY · UT PROSIM

ULTRA SAFE NUCLEAR CORPORATION

NSF

NECPHON 2017 A SUCCESS!

LOCAL COMPUTATIONAL PHONOLOGISTS MEET AT IACS

The 11th annual Northeast Computational Phonology (NECPhon) meeting took place at the Institute for Advanced Computational Science (IACS) at Stony Brook University on October 21. Over 30 local phonologists gathered to investigate basic principles and models regarding how sound systems in natural languages are represented, organized, learned, and change over time. This informal gathering was organized by IACS Professor Jeffrey Heinz from the Linguistics Department. "Over the past 11 years, NECPhon has been a great way to encourage linguists to learn about and develop computational methods for understanding the unconscious rules and constraints people use in every language across the world when they talk," said Heinz.
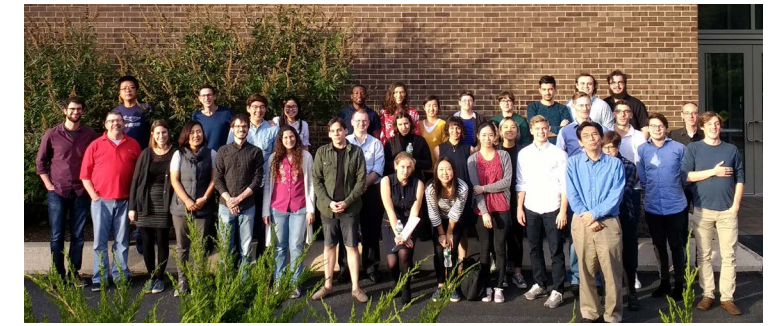
Examples of some of the topics discussed at the meeting are:

• syntax in phonology
• learning biases in opaque interactions
• acoustic categorization of Japanese vowel length
• subsequential steps to unbounded tonal plateauing.

Attendees hailed from SBU, University of Massachusetts Amherst, the University of Maryland, Rutgers, and Massachusetts Institute of Technology.

To learn more about NECPhon, you can visit http://blogs.umass.edu/comphon/meetings/necphon/.

THANK YOU

It has been another very successful year at the institute, and we owe much of our success to our supporters and benefactors. Without their backing, we would not be able to reach our goals or have the luxury of brainstorming new paths forward in our pursuit to bring computational science to the larger community.

As a result of the endowment and other support, in 2017 we accomplished the following:

• Supported travel for five national and international students and faculty to visit the Institute
• Hosted 17 speakers in our seminar series
• Completed our third annual IACS Computes! high-school summer camp program for 16 students
• Hired two new core faculty from Ecology & Evolution, and from Materials Science and Chemical Engineering
• Held seven programming workshops and our annual scientific writing course
• Awarded six Junior Researcher Awards; six Young Writer Awards, and eight Travel Awards
• Ran our first Research Experience for Undergraduates entitled Data + Computing = Discovery, with support also from the National Science Foundation, the Provost's Office, the College of Engineering and Applied Sciences, and the Office of the Vice President for Research
• With funding from the CIO's office, we hired our first group of students to form the HPC Support Team

• With funding from the CIO's office, we supported research computing across campus
• Hired student staff to help with event organization and overall administrative needs
• Contributed to the startup packages for new faculty
• Maintained annual support of the Center for Inclusive Education
• Enabled staff to take off-campus professional development courses
• Sent students as IACS ambassadors to recruiting venues across the nation
• Joined Software Carpentry as a silver member

Future goals are:

• Finish the recruiting and installing of our two endowed chair positions
• Officially register and advise advanced graduate Certificate in Data and Computational Science students
• 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

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iACS FACULTY

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*, 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.

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.

Rezaul Chowdhury

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

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.

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.

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

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.
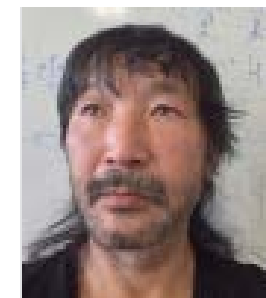
Hideo Sekino

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 Assocation http://n-as.org/ and he runs 'Rakudoan', a performance art space in Tokyo http://n-as.org/rakudoan/index.htm".

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.

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 additions 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.

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11. Mahdi Davari
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36. Bryan Sundahl
37. Xuebin Wang
38. Yulun Wang
39. Donald Willcox
40. Oliver Yang
41. Casey Youngflesh
42. Wei Zhang
43. Yang Zhang
44. Xin Zhou
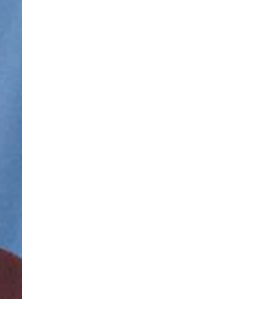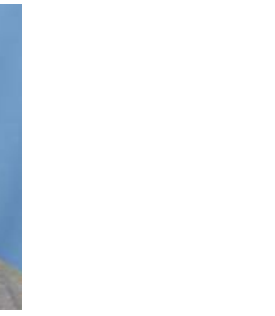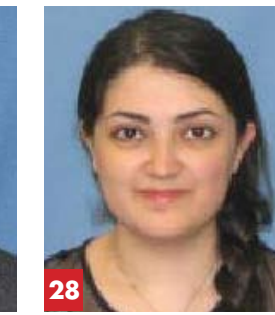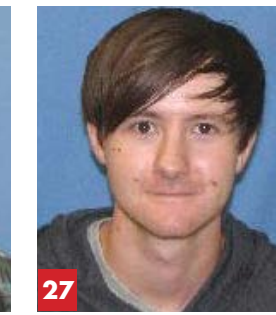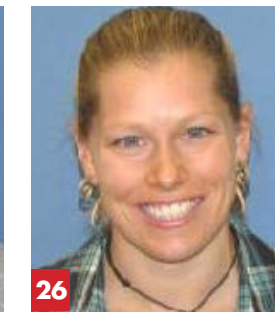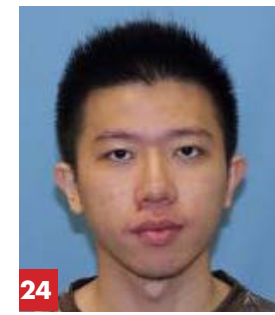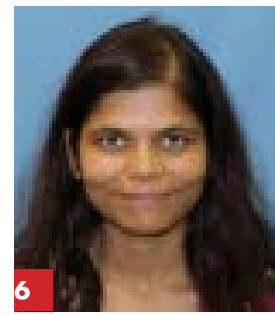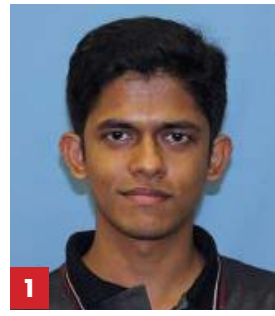
ALUMNI

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PhD, Applied Mathematics & Statistics 2017
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PhD, Physics & Astronomy 2016
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Solutions Architect, NVIDIA

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PhD, Applied Mathematics & Statistics 2016
Applied Scientist, Amazon

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PhD, Computer Science 2016
Research Scientist, Google

9. Jesmin Jahan Tithi
PhD, Computer Science 2015
HPC Software Architect, Intel Corporation

10. Na Zhang
PhD, Applied Mathematics & Statistics 2015
Technical Staff, VMWare

POLAR HACKATHON

Associate Professor Heather Lynch, an IACS faculty member, and visiting professor Shantenu Jha, led a week-long software carpentry workshop and polar science hackathon at IACS in August 2017. Over the course of the week, 26 polar scientists and research programmers from as far away as Alaska and Norway gathered together to tackle a range of computing intensive projects ranging from ice-river monitoring to permafrost modeling to mapping seals using satellite imagery. Other highlights included a Google-led workshop on TensorFlow and sessions on Open Science Grid and reproducible research.
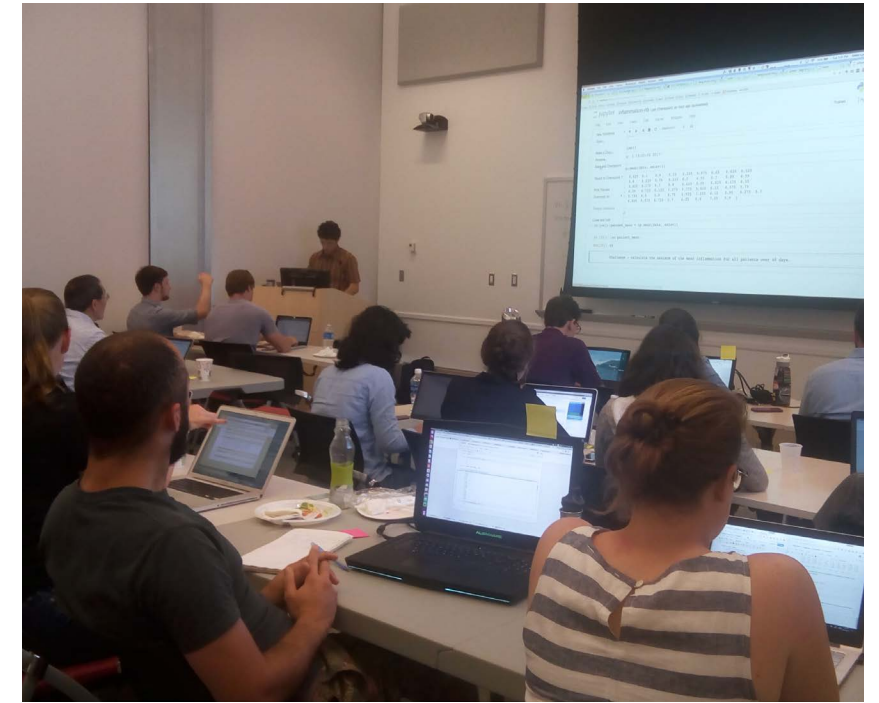
13TH ANNUAL IWOMP CONFERENCE HELD AT SBU

The International Workshop on OpenMP (IWOMP) is an annual workshop dedicated to the promotion and advancement of all aspects of parallel programming with OpenMP. It is the premier forum to present and discuss issues, trends, recent research ideas, and results related to OpenMP.

The 13th annual workshop took place at Stony Brook University on September 18-20. IACS Professor Barbara Chapman and members of her research group were the lead organizers of the conference, which featured papers and presentations of previously unpublished technical work detailing innovative, original research and development related to OpenMP. The conference was attended by 50 people.
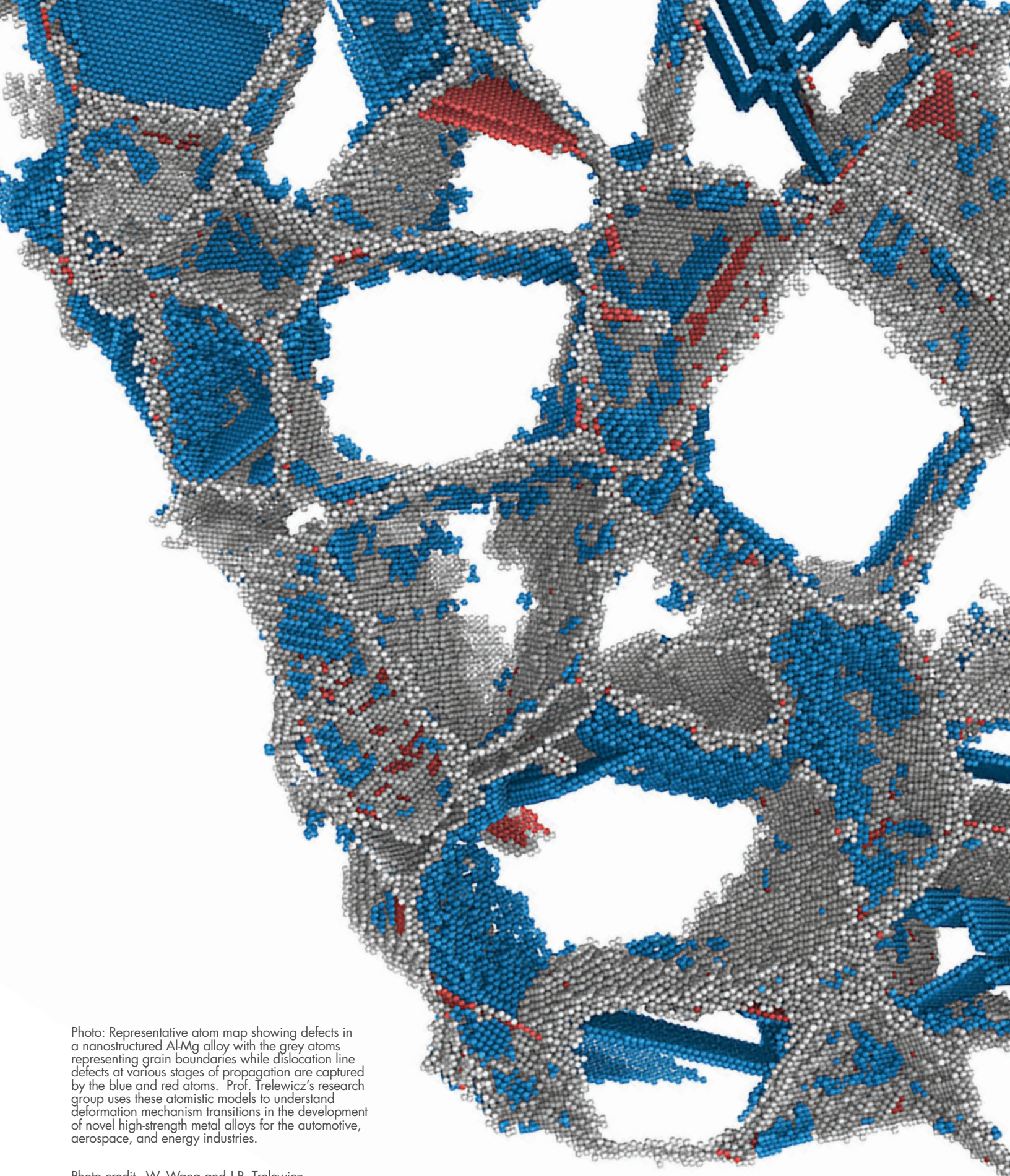
Photo: Representative atom map showing defects in a nanostructured Al-Mg alloy with the grey atoms representing grain boundaries while dislocation line defects at various stages of propagation are captured by the blue and red atoms. Prof. Trelewicz's research group uses these atomistic models to understand deformation mechanism transitions in the development of novel high-strength metal alloys for the automotive, aerospace, and energy industries.

Photo credit - W. Wang and J.R. Trelewicz